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Danish in-kind simulation efforts to the ESS - an overview

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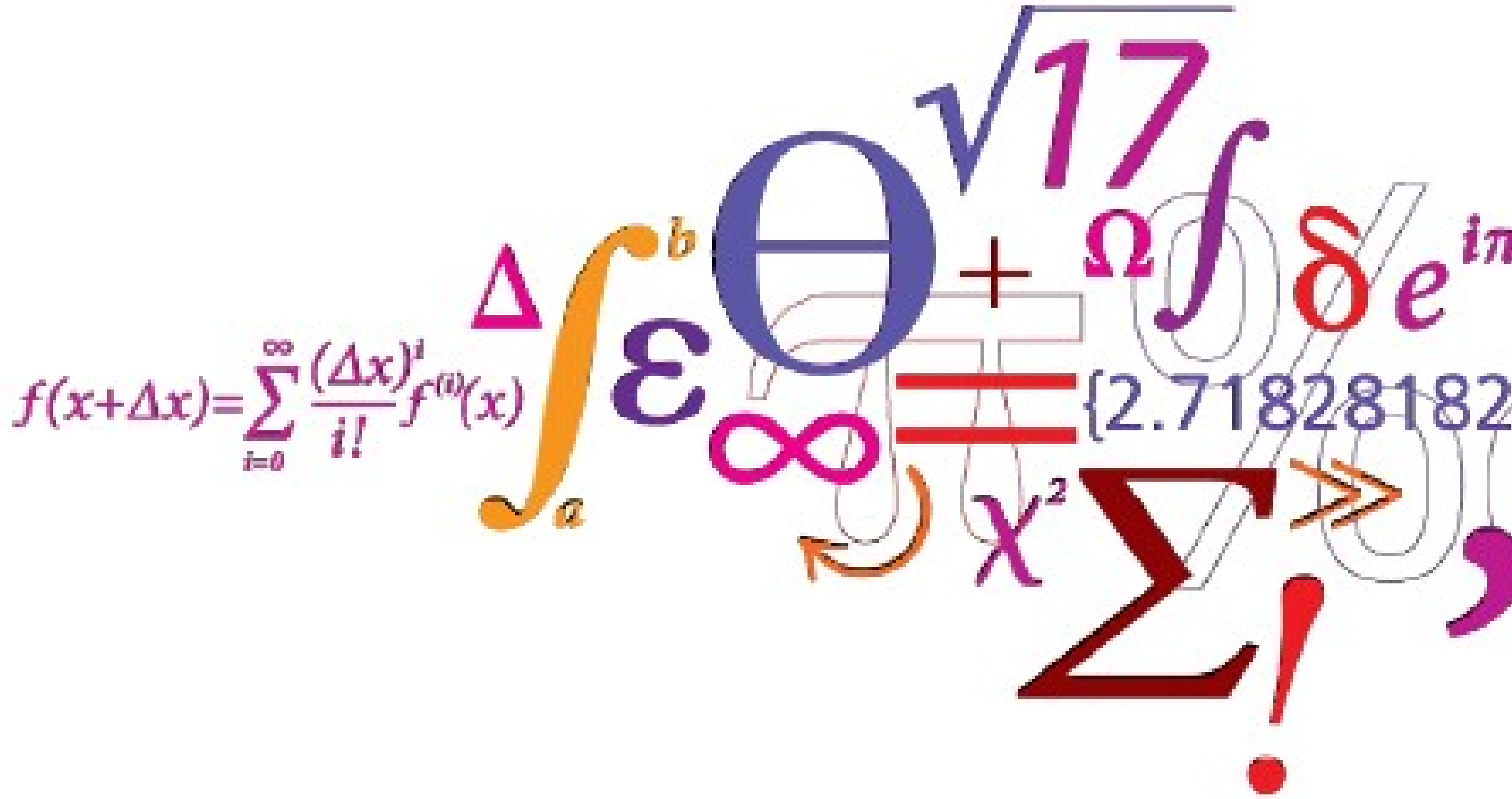
Danish in-kind simulation efforts to the ESS
- an overview

Esben Klinkby, DTU Nutech

contributions from:
Peter Willendrup (DTU)
Kim Lefmann (Uni Copenhagen)



DTU Nutech
Center for Nukleare Teknologier

EUROPEAN SPALLATION SOURCE

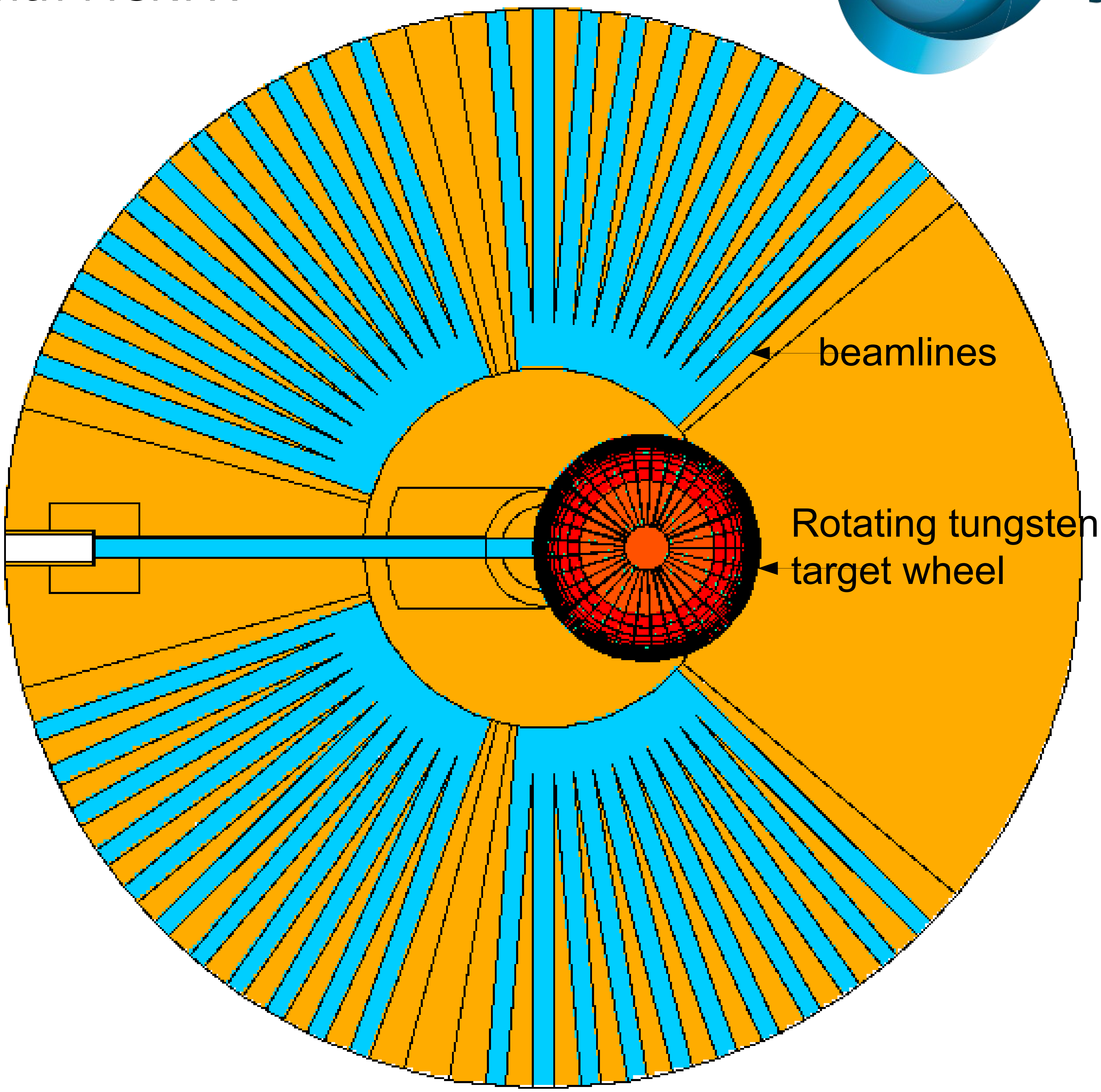
Outline

- From hard protons to cold neutrons
  - Experimental overview
  - Simulation tools
  - “*In house”* simulation efforts
- “*In country*“ instrument design

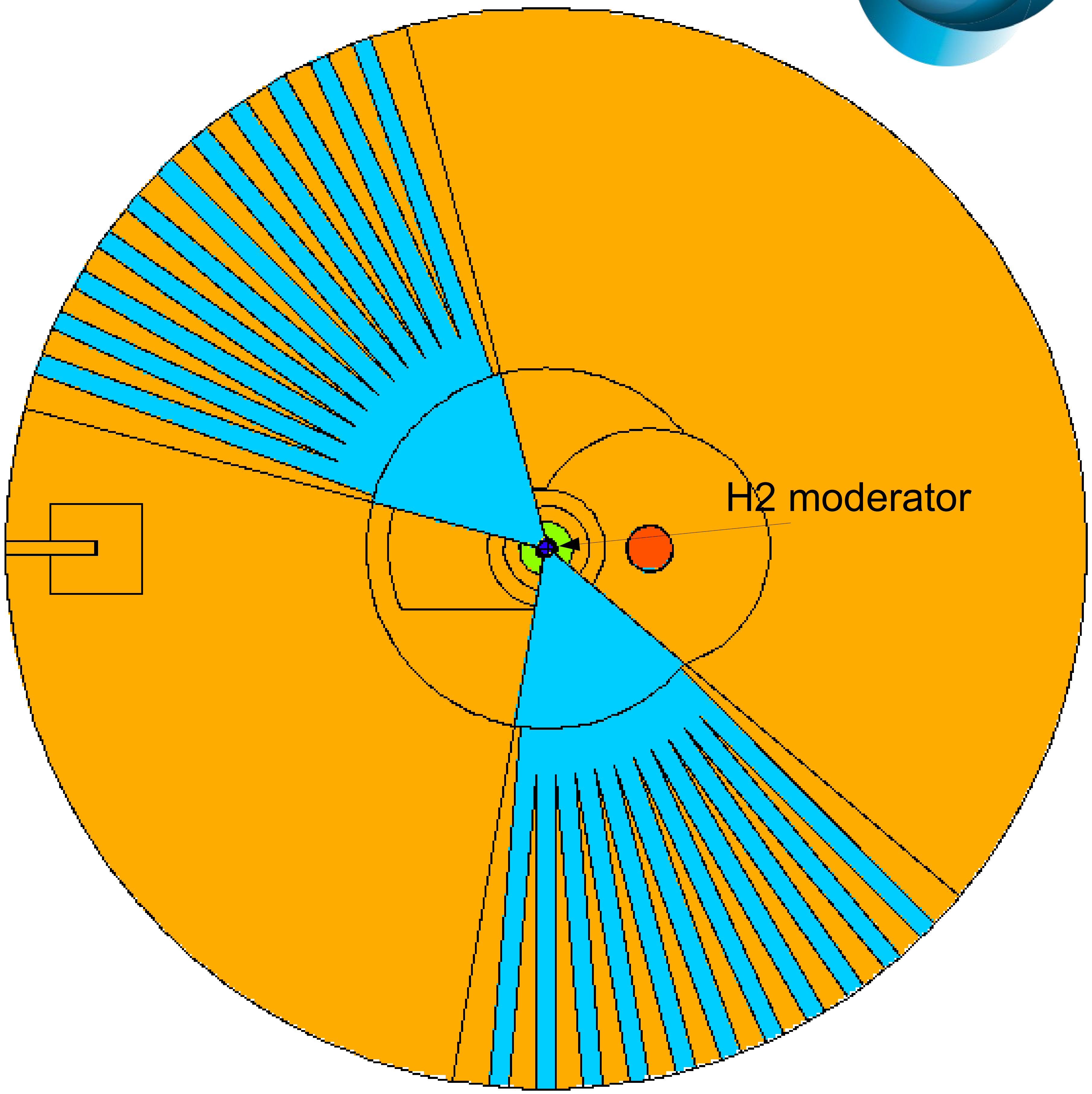
Risø

Target station design

- Target station modeled with MCNPX
- Spallation takes place in rotating tungsten target
- The scale of the objects under study dictates the the use of cold neutrons (~1-10meV)
- Neutrons are moderated in H_2 and H_2O for cold and thermal neutrons



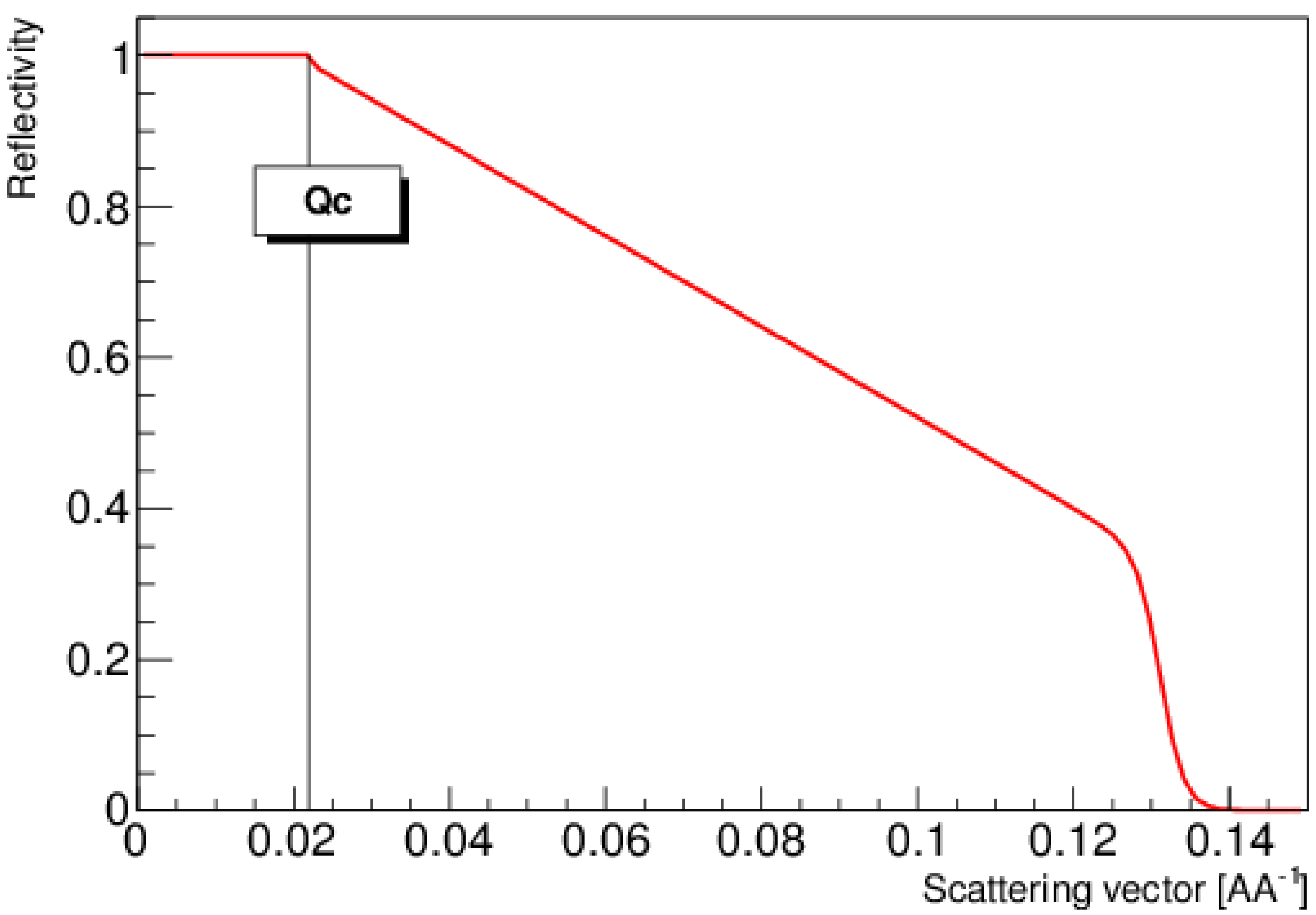
Flip-view



Neutron guides

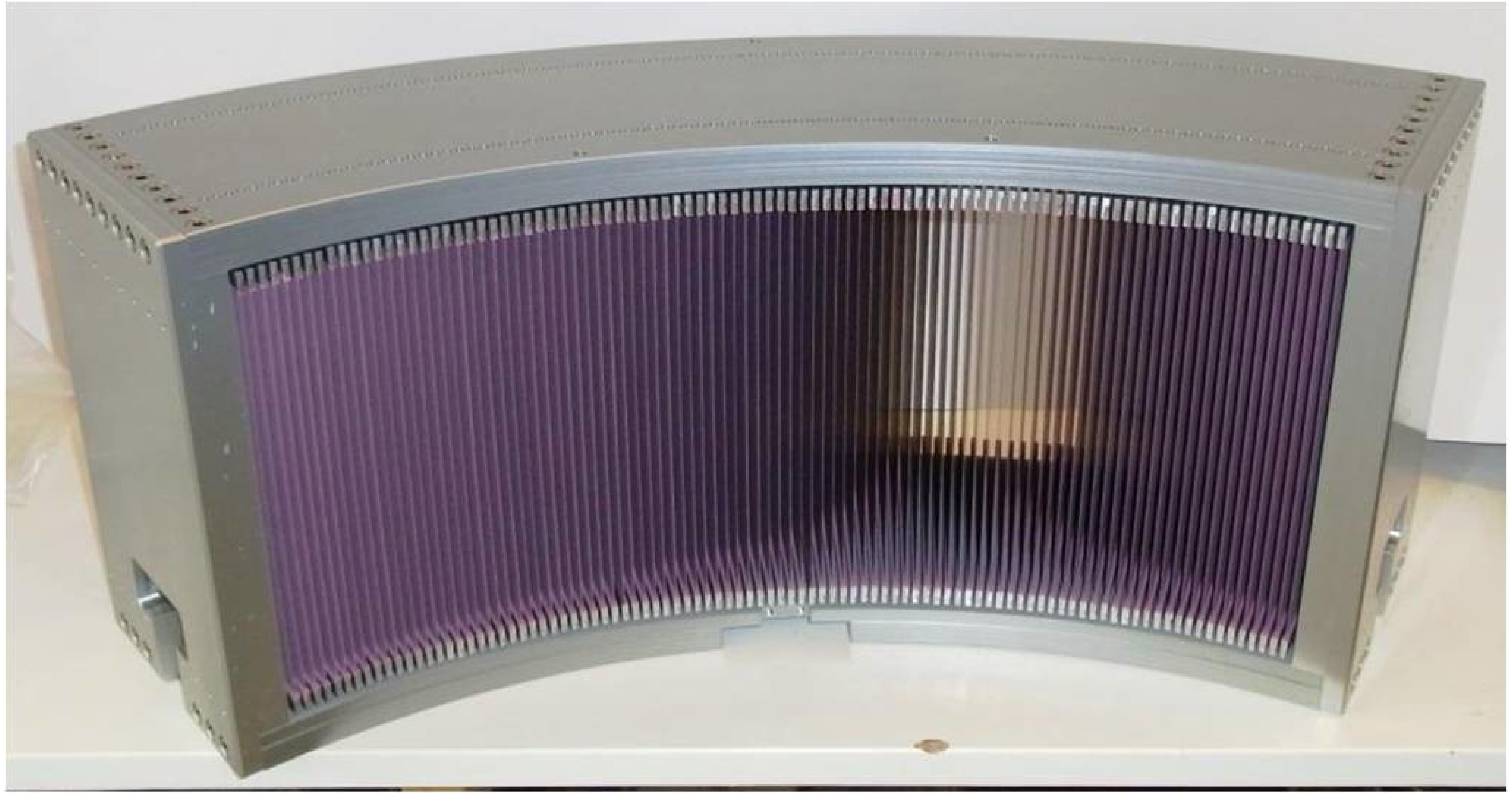
- Ni and Ti are chemically similar, but have very different refraction indices
- Coating with alternating layers:

  "Supermirrors" of which guides can be built which ~without loss, transport cold neutrons to radiation safe distances allowing ToF to be measured



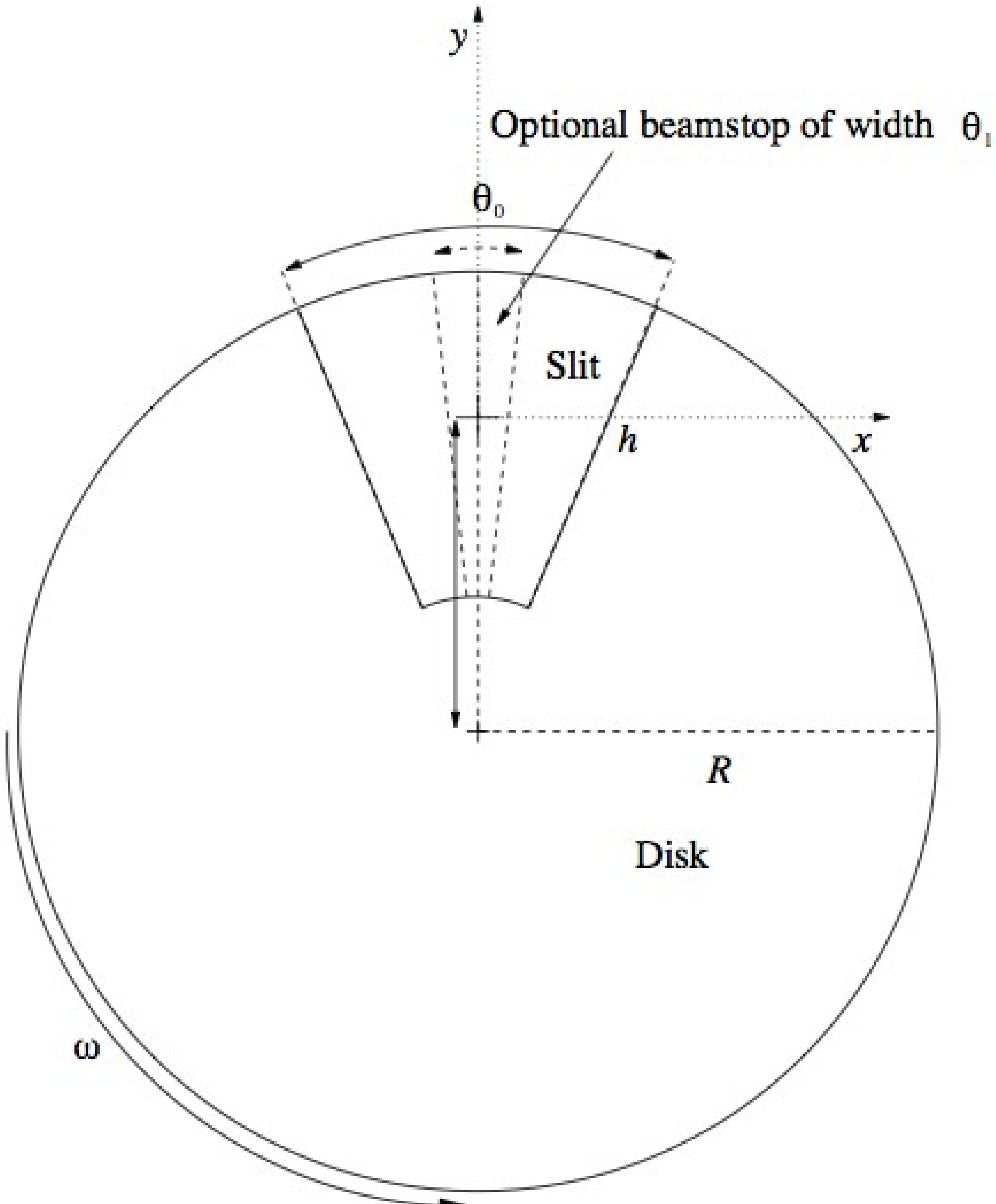
Collimators & slits

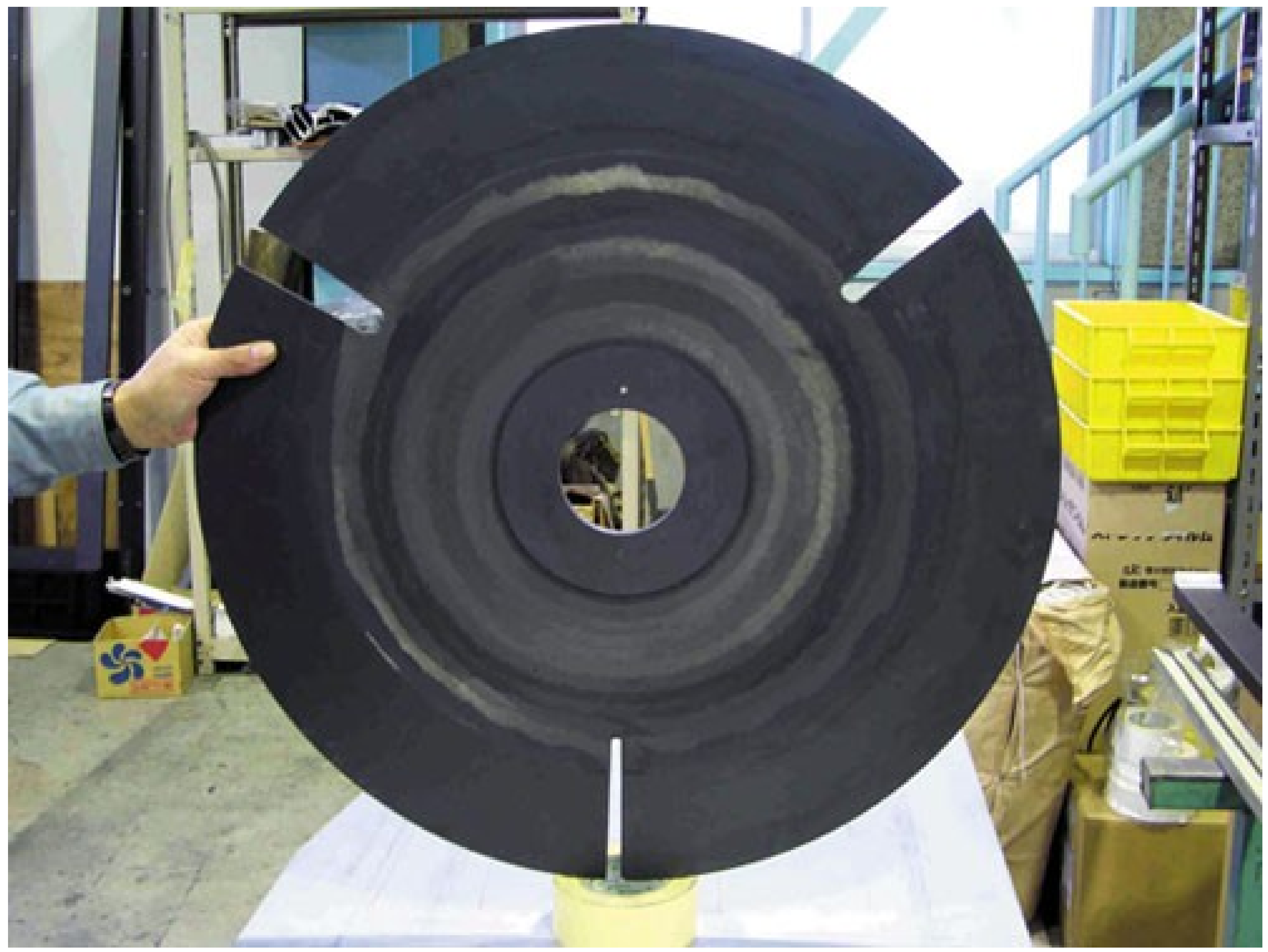
- Works from the principle: Absorb anything which don't have the desired direction (gadolinium)
- Discriminate beam in *space* and *divergence*



Disk Choppers

- Introduce pulses
- Discriminate beam in *time*
- Combining two choppers ~ Fermi chopper / velocity selector



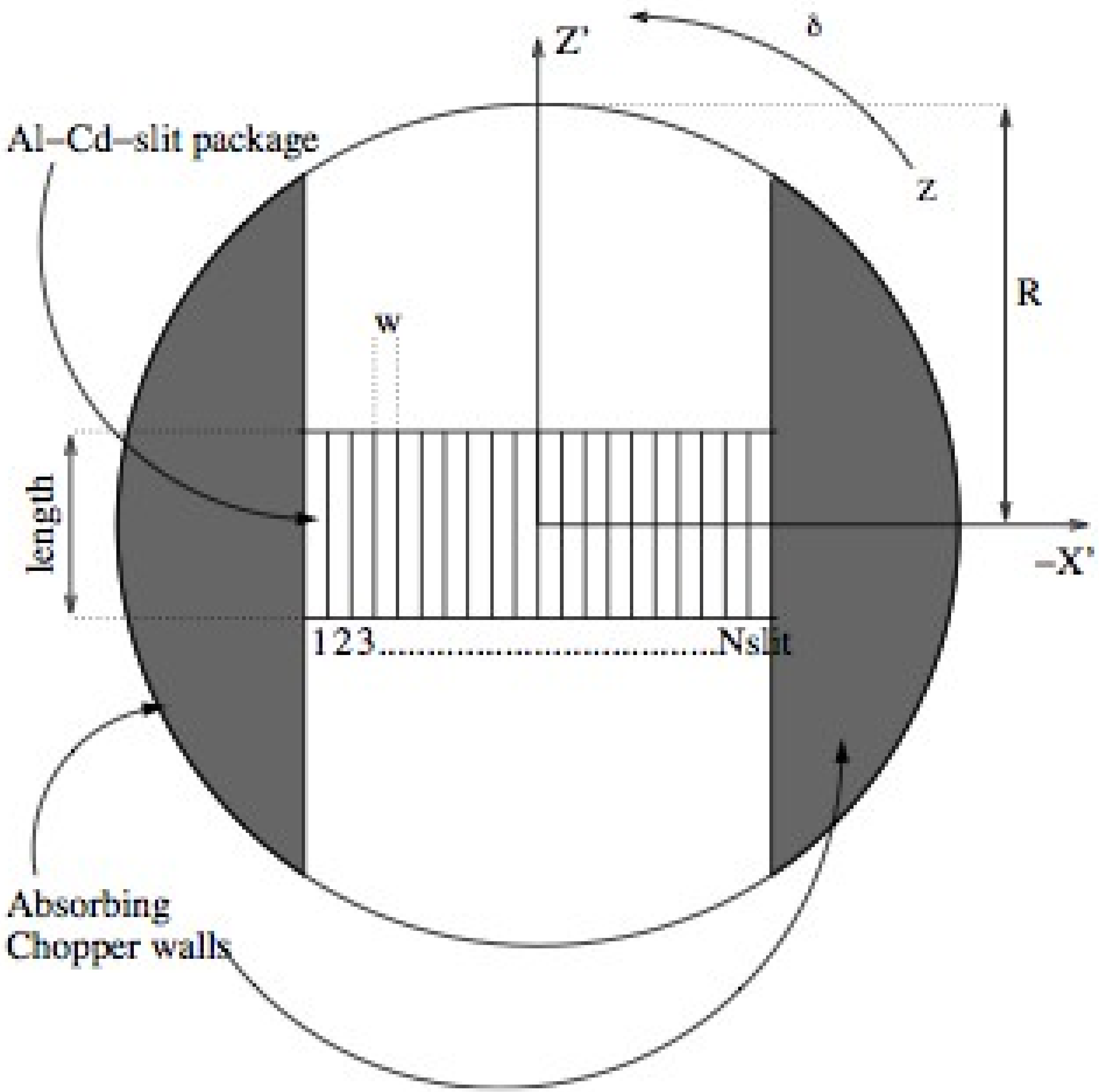


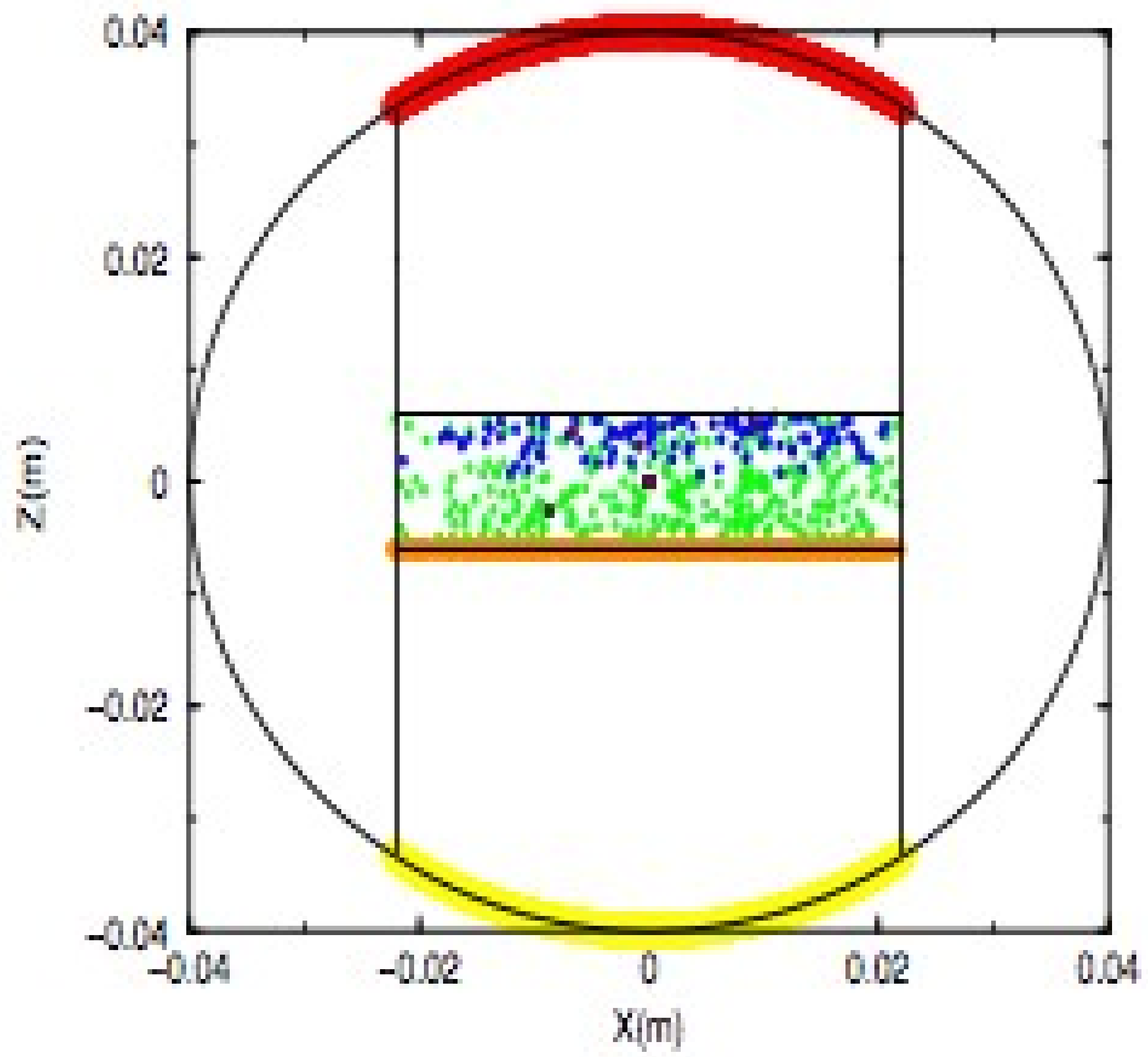
Velocity selector

- Discriminate beam in *velocity* / *wavelength*
- $\Delta\lambda/\lambda \sim 10\%$

Fermi Choppers

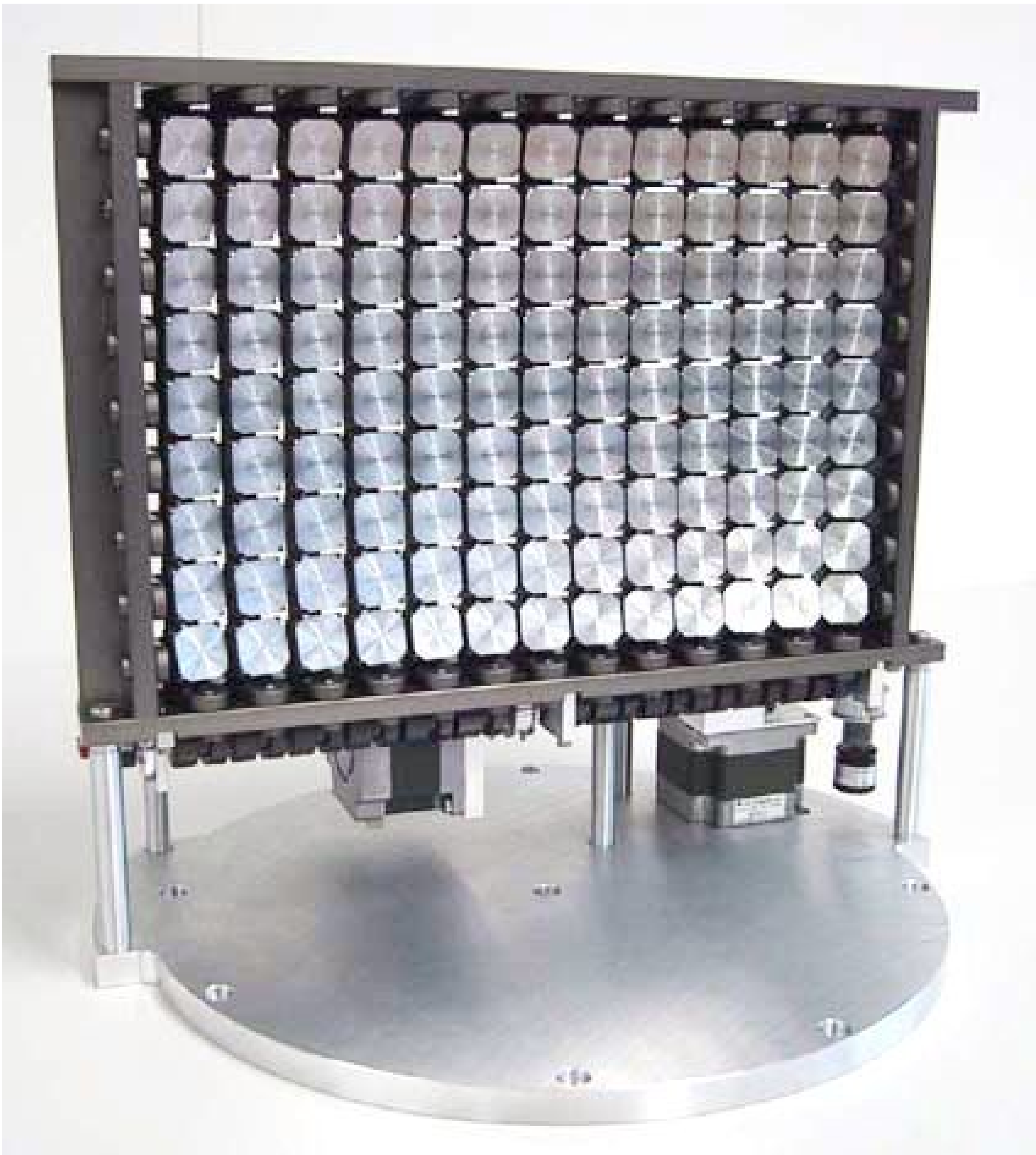
- Discriminates beam in *time* and *wavelength* simultaneously

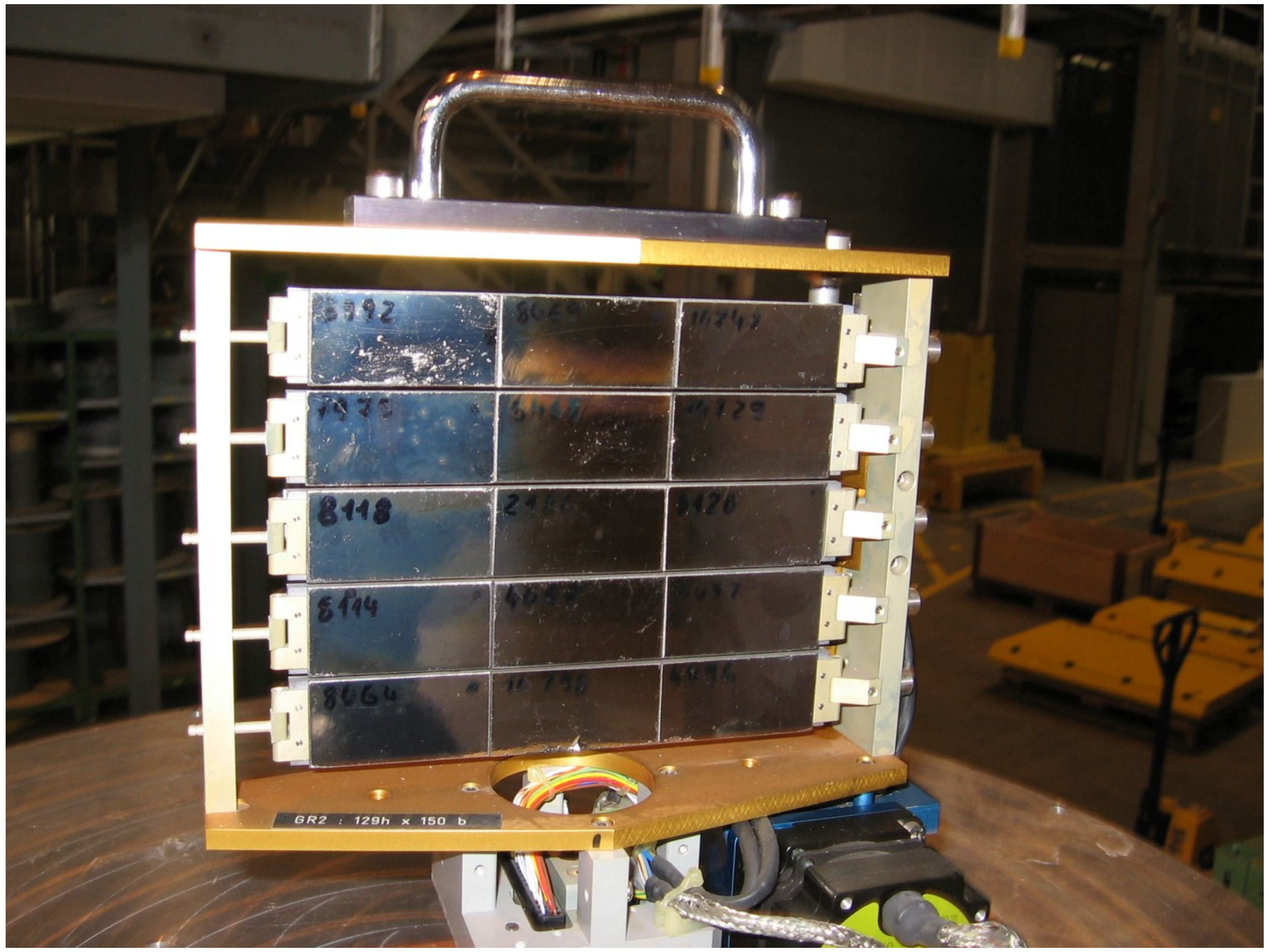




Crystal monochromators (and analyzers)

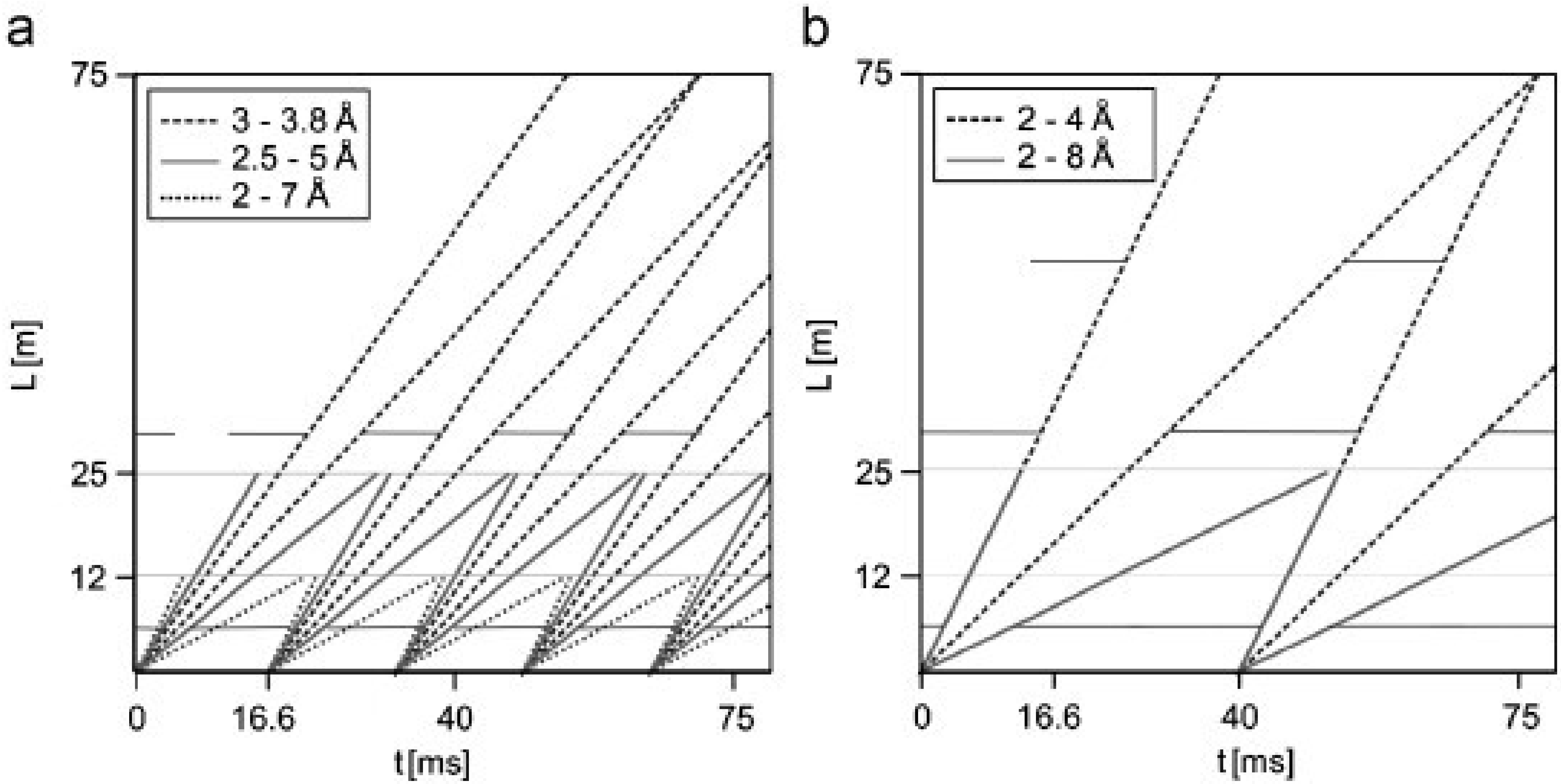
- Discriminate beam in *wavelength* by Bragg's law
- $\Delta\lambda/\lambda$ ~ 1% (plus multiples $\lambda/2$, $\lambda/3$, ...)





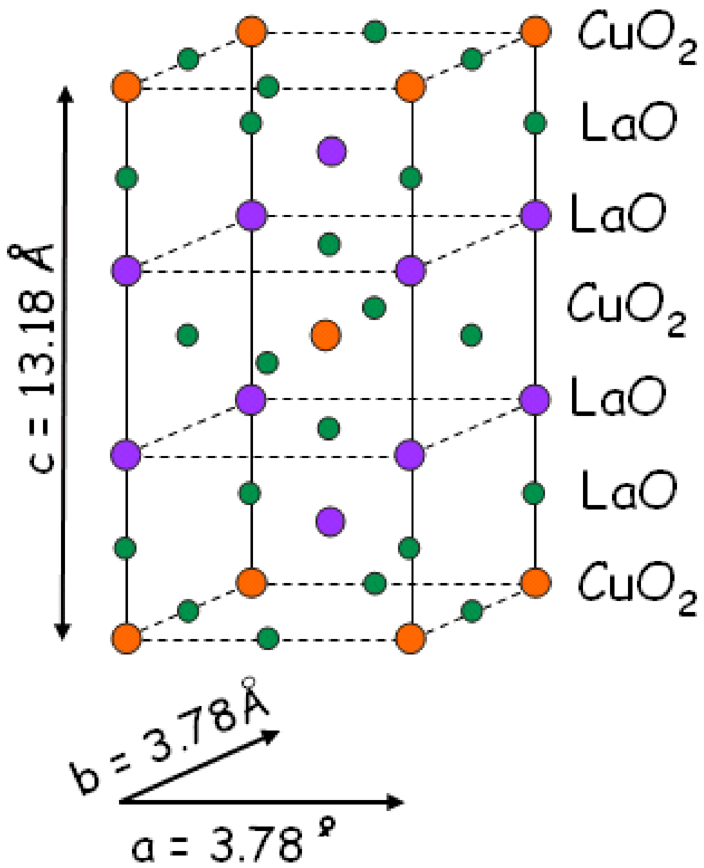
Beamline design

- By a suitable selection of: choppers, velocity selectors etc etc the neutron scatterer is able to 'design' the beam optimal for his/her sample.

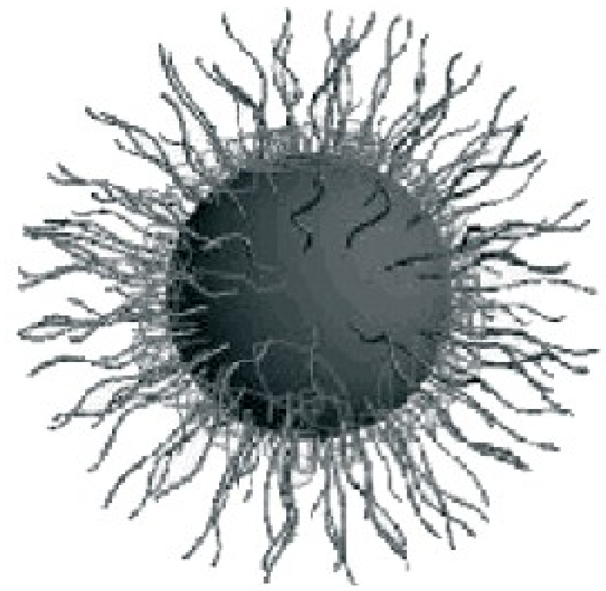


Some samples studied

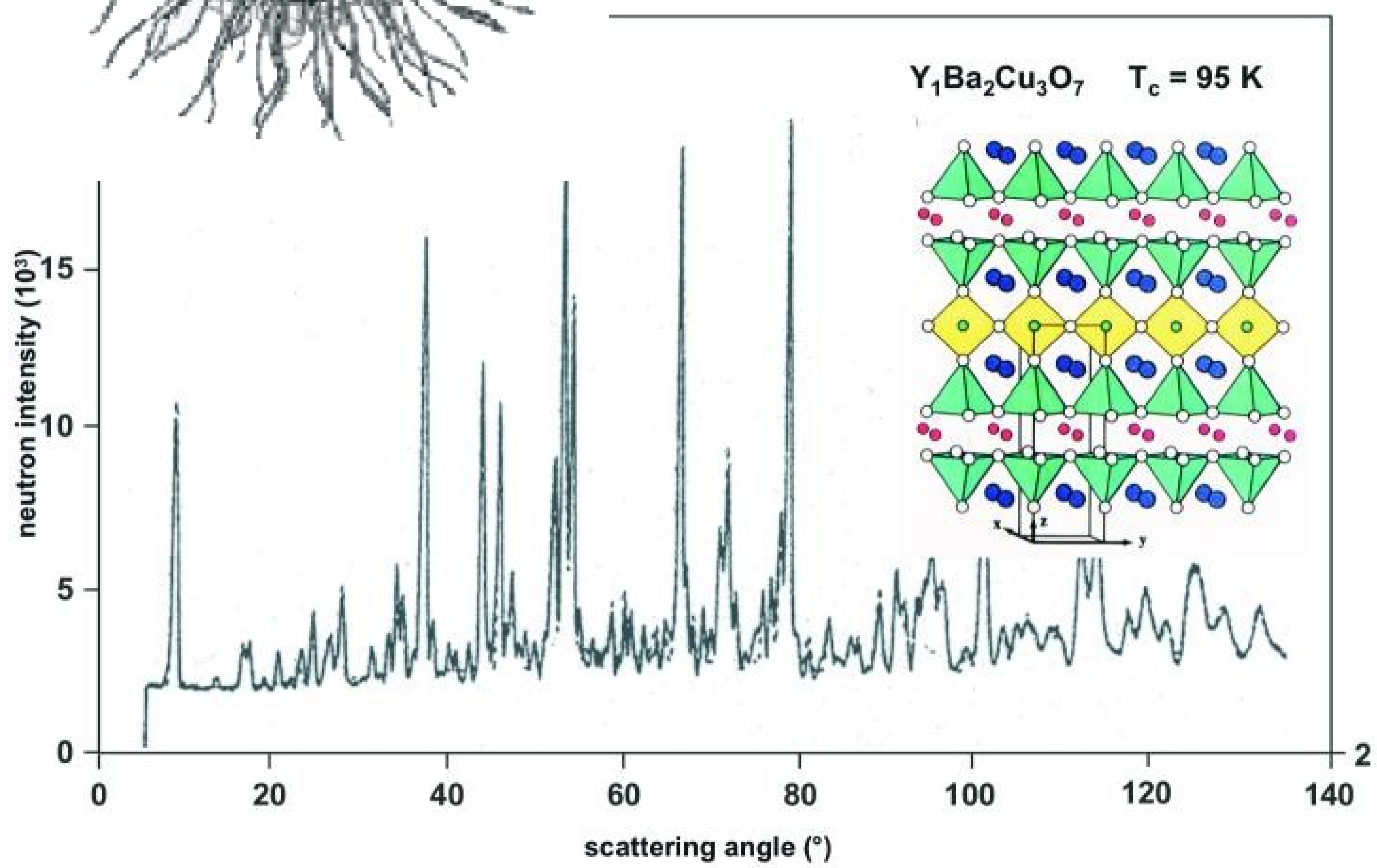
- Numerous, cross-disciplinary



- Materials in different states, eg.
  - Crystals
  - Powders
  - Molecules in solution



- Materal behaviour/function
  - Materials for
  fuel cells, batteries...
  - Magnets
  - Superconductors
  - Chemical reactions
  - Protein folding
  - Polymers
  - Metallurgy
  - ...



- Å to m distances
- Fourier (reciprocal space) methods
- Direct space methods

Detectors

- Since neutrons are electrically neutral, they are difficult to detect.
- The preferred reaction is:

$$n + {}^{3}He \rightarrow {}^{3}H + p$$

due to the high cross-section

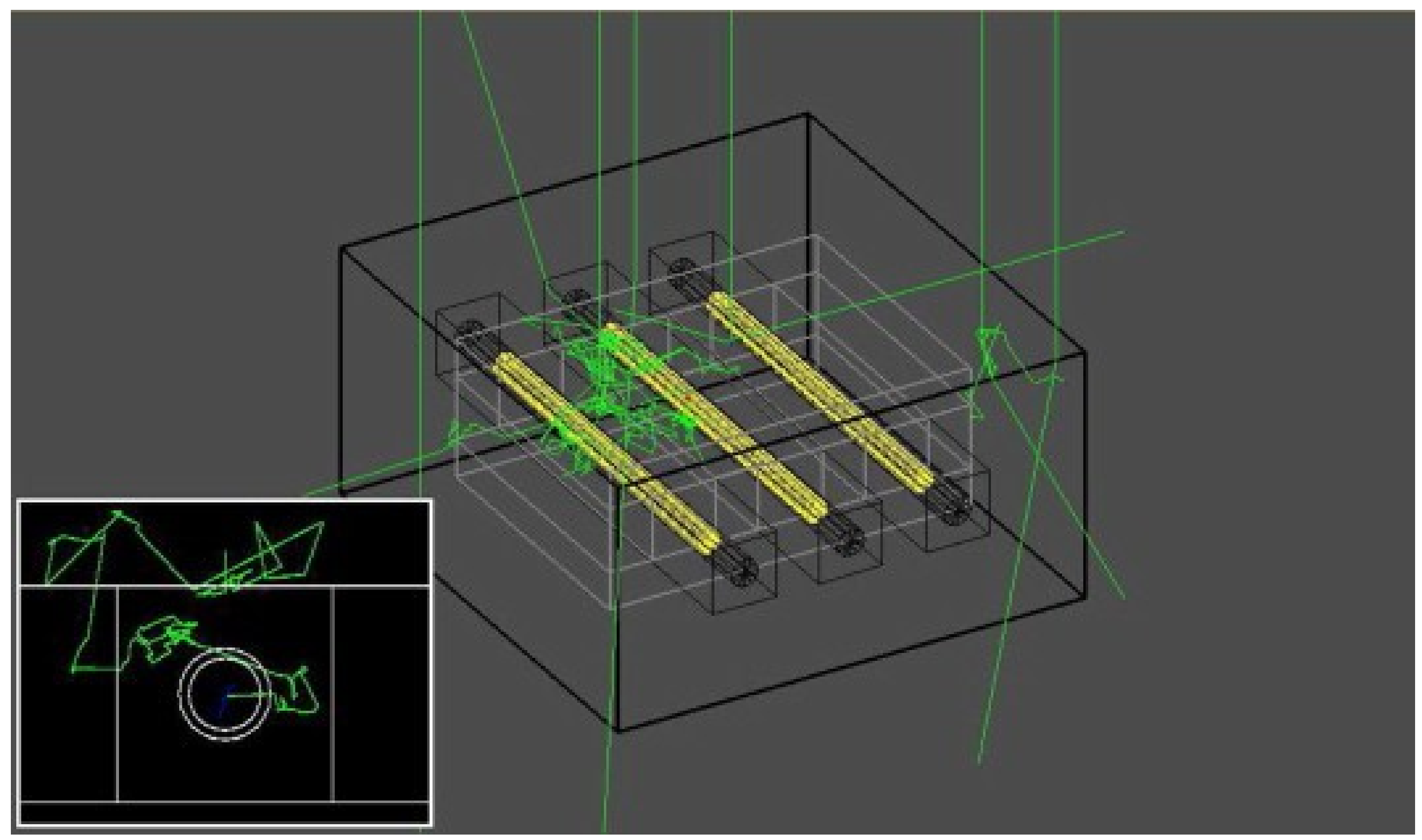
E field → protons collected → signal

- Recent years lack of ${}^{3}He$ has forced the community to look for alternatives:

$$n + {}^{10}B \rightarrow {}^{7}Li + {}^{4}He\,.$$

due to the high neutron capture cross-section of ${}^{10}B$

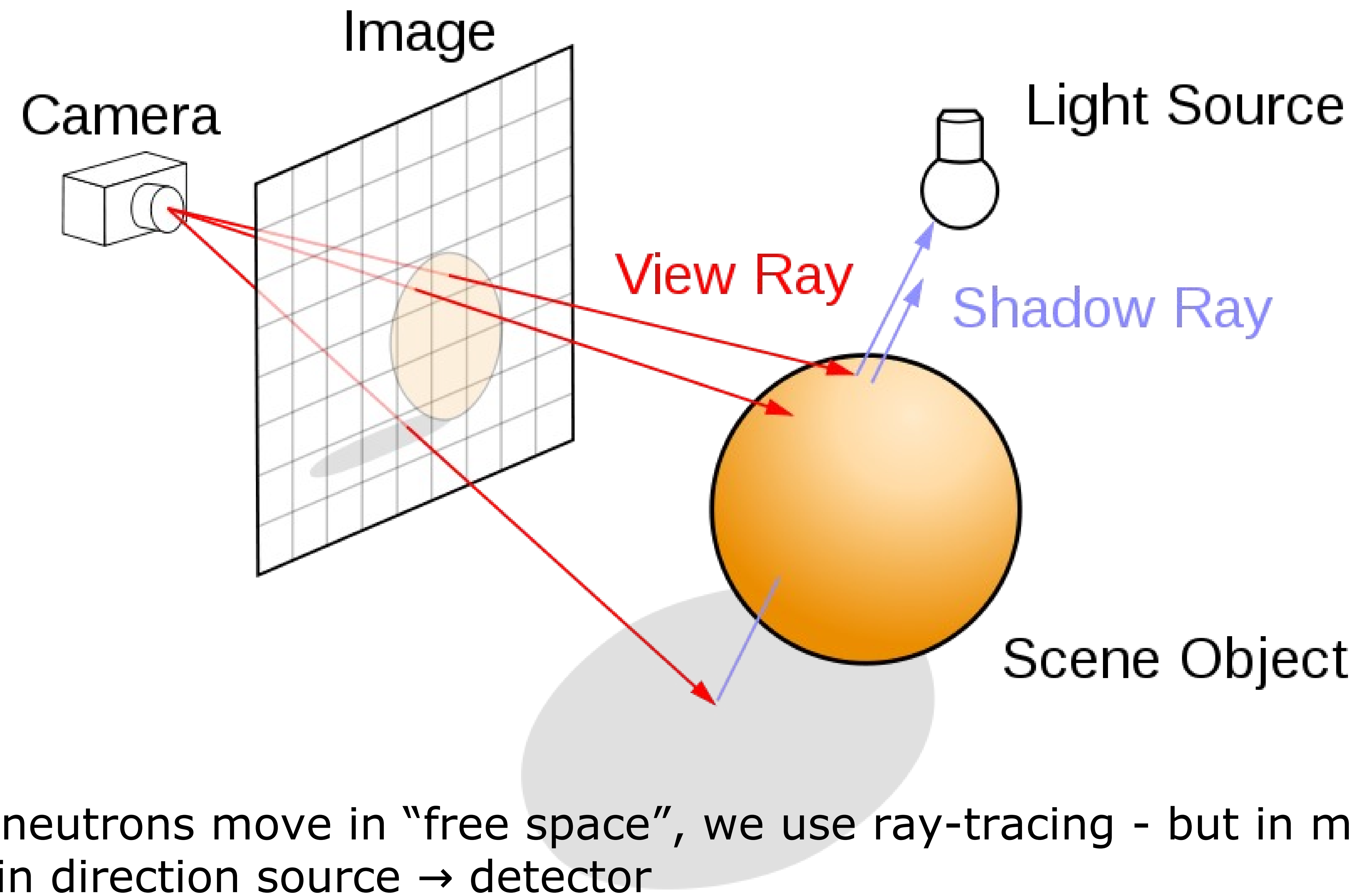
The energetic nuclei ionize gas molecules which can be collected as signals



Monte Carlo techniques

- Los Alamos has since then developed and perfected many different monte carlo codes leading to what is today known as the codes MCNP5 and MCNPX
- State of the art is MCNPX (or soon the merged MCNP6 code) that features numerous (even exotic) particles
- MCNP was originally Monte Carlo Neutron Photon, later N-Particle
- Mainly used for high-energy particle descriptions in weapons, power reactors and routinely used for estimating dose rates and needed shielding
- Does not to date handle coherent scattering of neutrons due to the focus on high energies

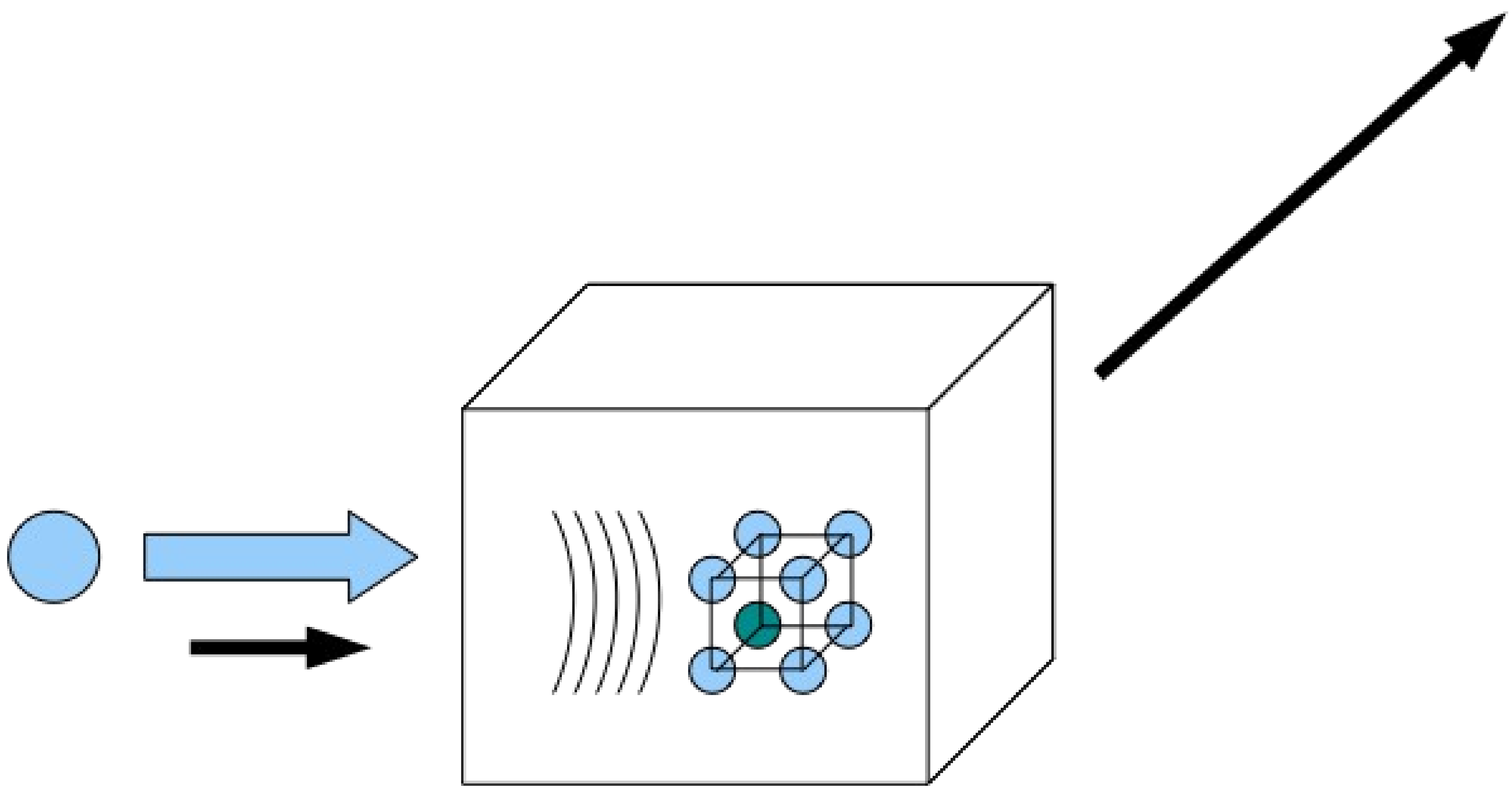
Ray-tracing methods



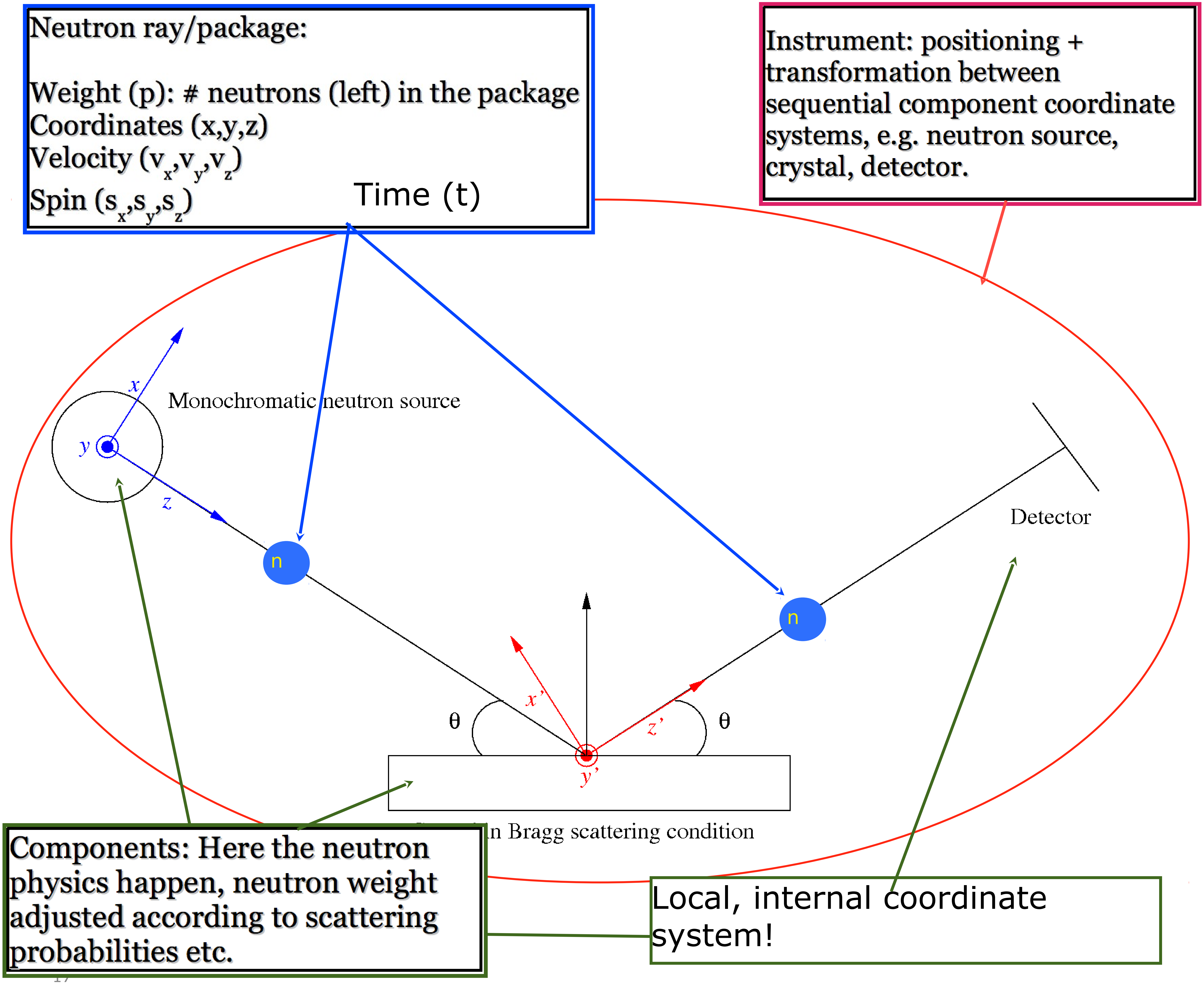
- When neutrons move in “free space”, we use ray-tracing - but in most cases in direction source → detector
- Of course parabolas rather than straight lines are uses to implement gravity

Elements of Monte-Carlo raytracing

- Instrument Monte Carlo methods implement coherent scattering effects
- Uses deterministic propagation where this can be done
- Uses Monte Carlo sampling of “complicated” distributions and stochastic processes and multiple outcomes with known probabilities are involved
  - i.e. inside scattering matter
- Uses the particle-wave duality of the neutron to switch back and forward between deterministic ray tracing and Monte Carlo approach

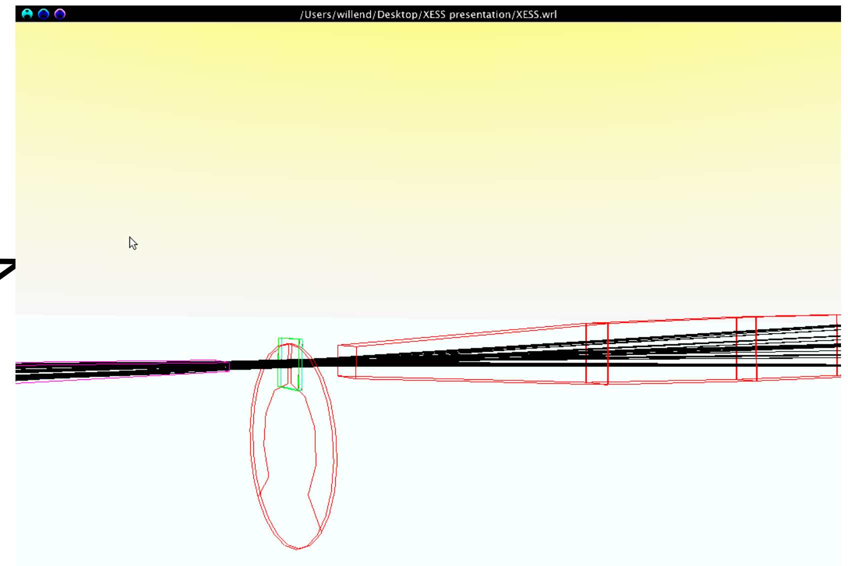


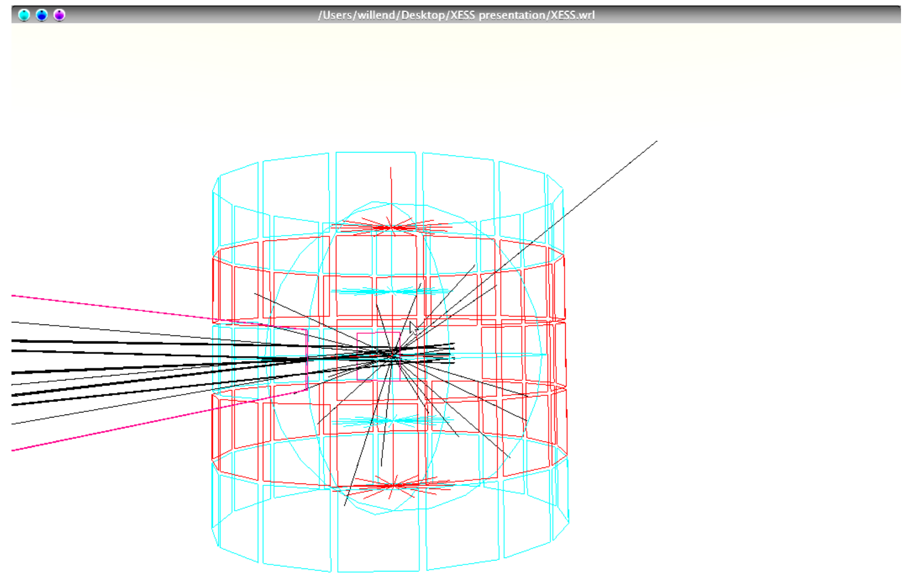
- Result: A realistic and efficient transport of neutrons in the thermal and cold range
- ***McStas***: the code (of Risø origin) that encompass transport, beam-line and detector simulation, analysis framework



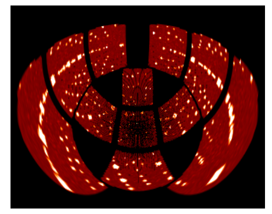
Neutron ray/package:
Weight (p): # neutrons (left) in the package
Coordinates (x,y,z)
Velocity (v_x,v_y,v_z)
Spin (s_x,s_y,s_z)
Time (t)
Instrument: positioning + transformation between sequential component coordinate systems, e.g. neutron source, crystal, detector.
x
y
z
Monochromatic neutron source
n
n
Detector
θ
θ
x'
z'
y'
n Bragg scattering condition
Components: Here the neutron physics happen, neutron weight adjusted according to scattering probabilities etc.
Local, internal coordinate system!

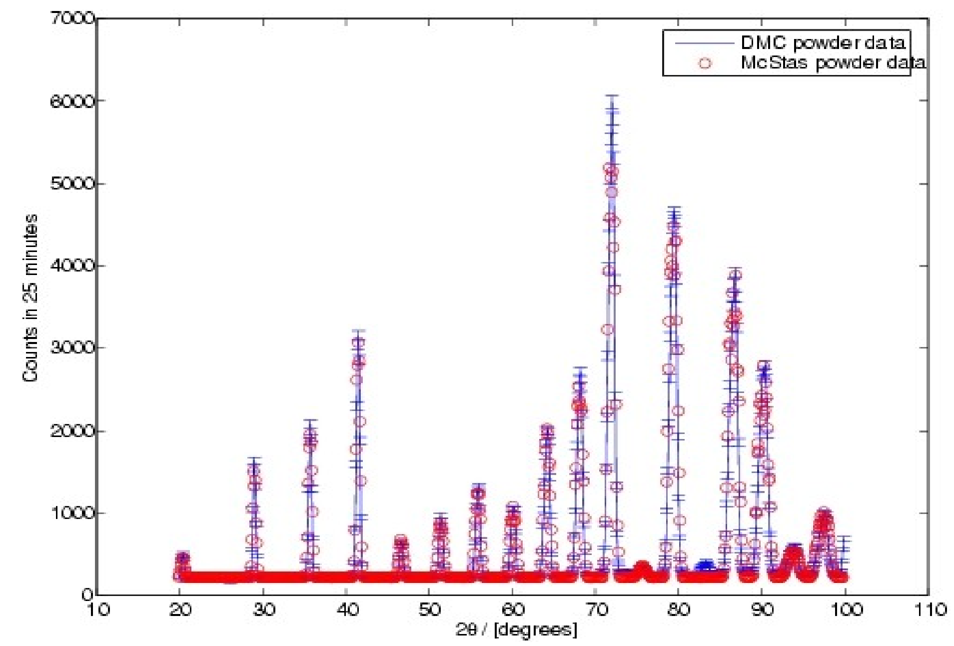
What is McStas used for?



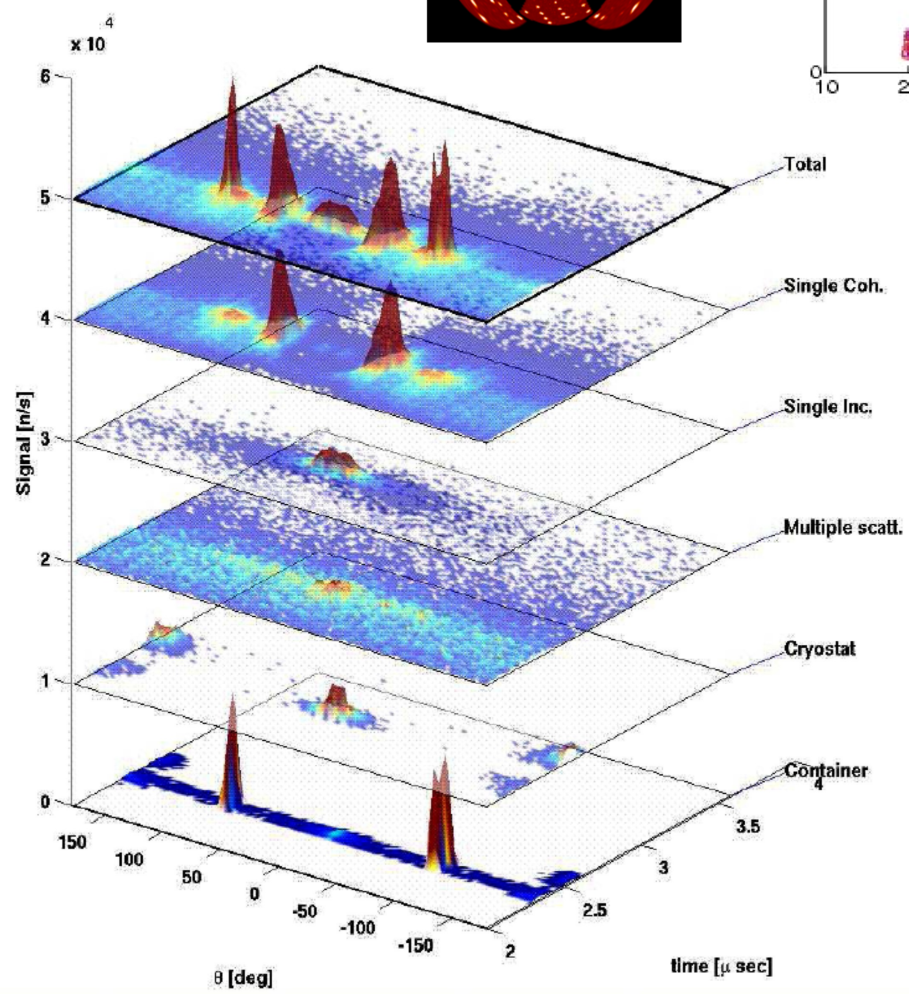


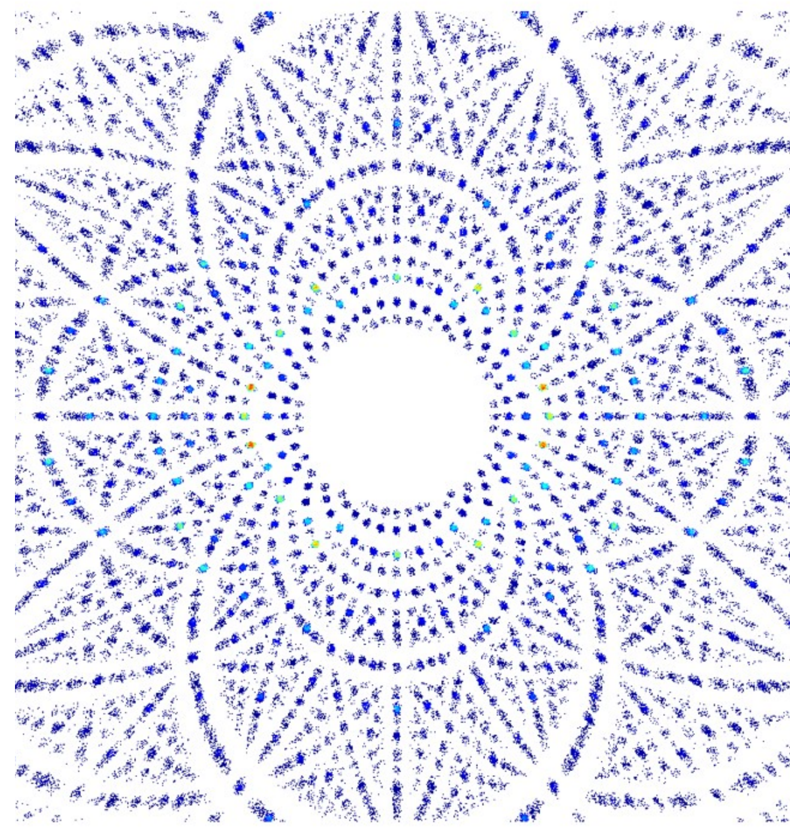
- Instrumentation
- Virtual experiments
- Data analysis
- Teaching

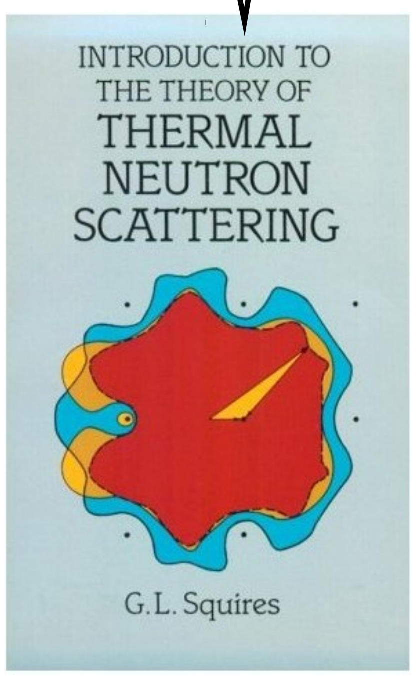


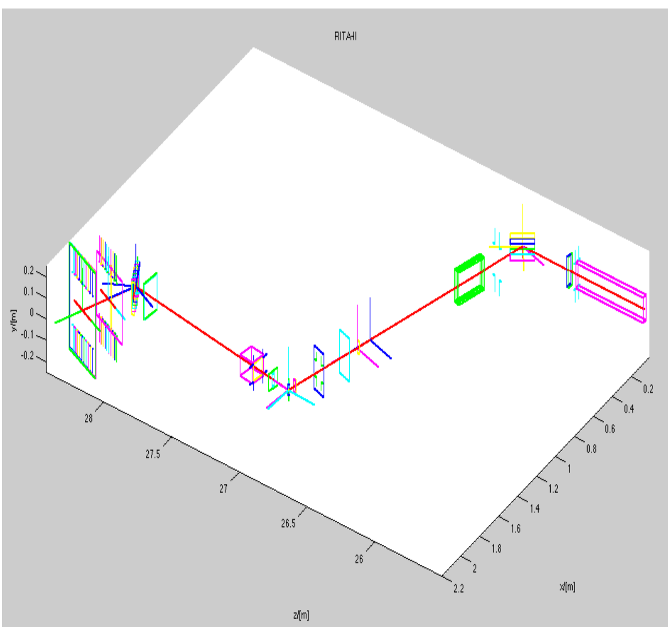


KU, DTU 2005-2012
INSIS, NIDS, ESS workshops

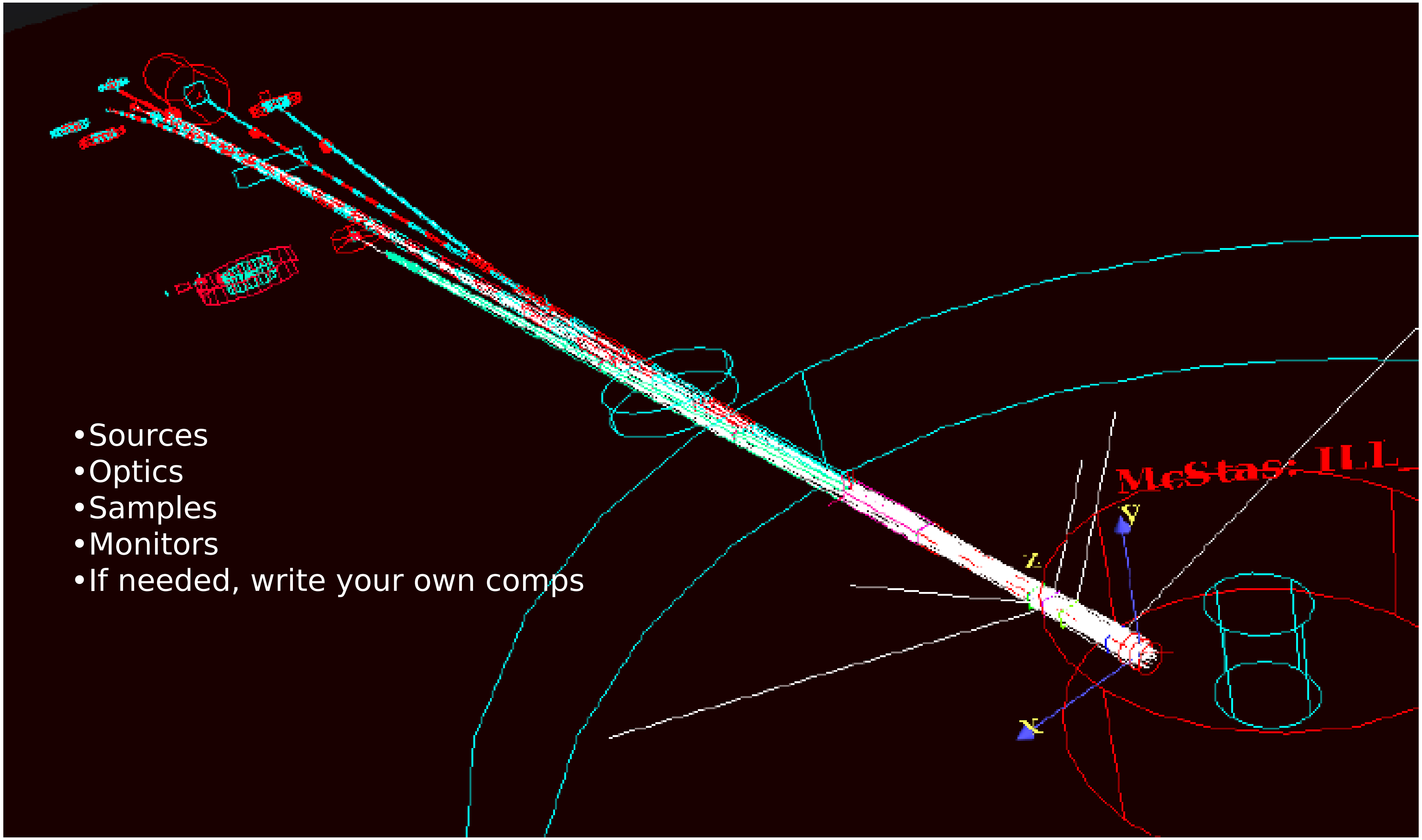








Example from ILL



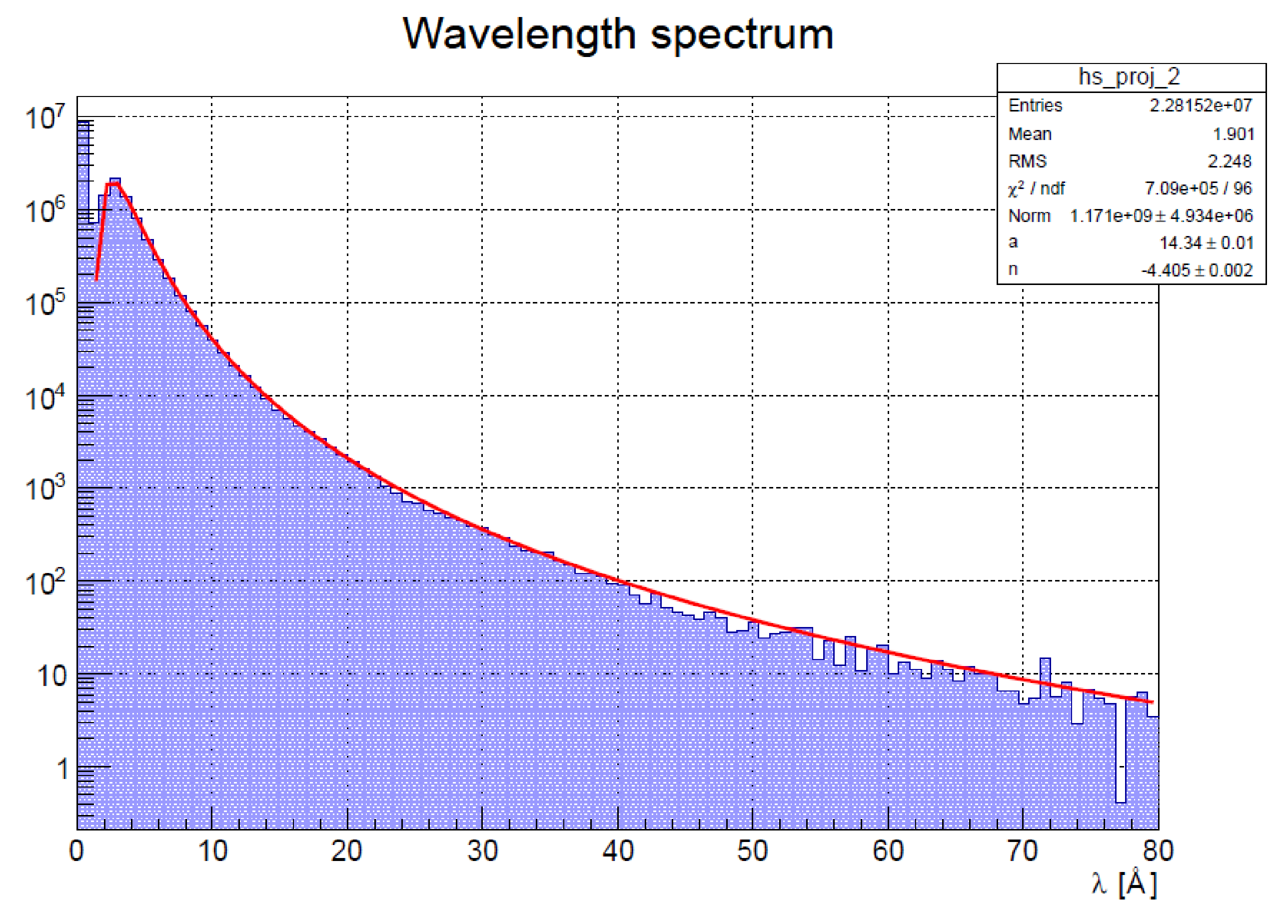
- Sources
- Optics
- Samples
- Monitors
- If needed, write your own comps

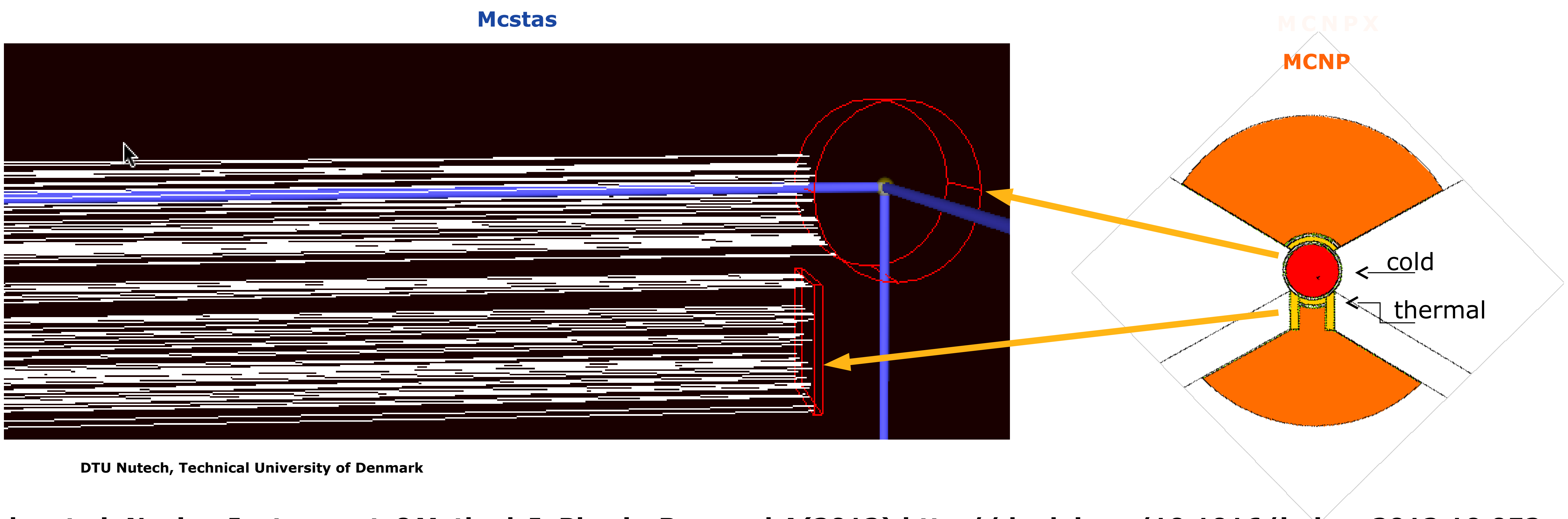
Example from ILL – E.Farhi

How to get from MCNPX to McStas

- Based on the latest MCNPX ESS target station (bi-spectral) geometry from ESS-Bilbao we have developed a McStas component mimicking both geometry and spectra.

- We are also working on alternatives which transport the neutron state directly, thus avoiding loss of phase-space / making assumptions





E.Klinkby,et al.,NuclearInstruments&MethodsInPhysicsResearchA(2012),http://dx.doi.org/10.1016/j.nima.2012.10.052

Danish in-kind contributions

- 1.0 M€. Proton beam control (Søren Pape Møller, AU)
- 1.5 M€. Data Management and Software Center (Stig Skelboe, KU)
- 1.0 M€. Instrument simulation central office (Kim Lefmann KU, P.Willendrup DTU)
- 0.1 M€. Integrating moderator- and instrument simulations
  (B.Lauritzen, P.Willendrup, E.Nonbøl, E.Klinkby DTU)

- 0.2 M€. Radio-ecology baseline (Mikael Jensen, Sven Nielsen DTU)
- 0.1 M€. MANTID – DMSC (Stig Skelboe, KU)
- 0.8 M€. 5 DK-CH instrument packages
  (Niels Bech Christensen, DTU; Christian Rüegg, PSI)

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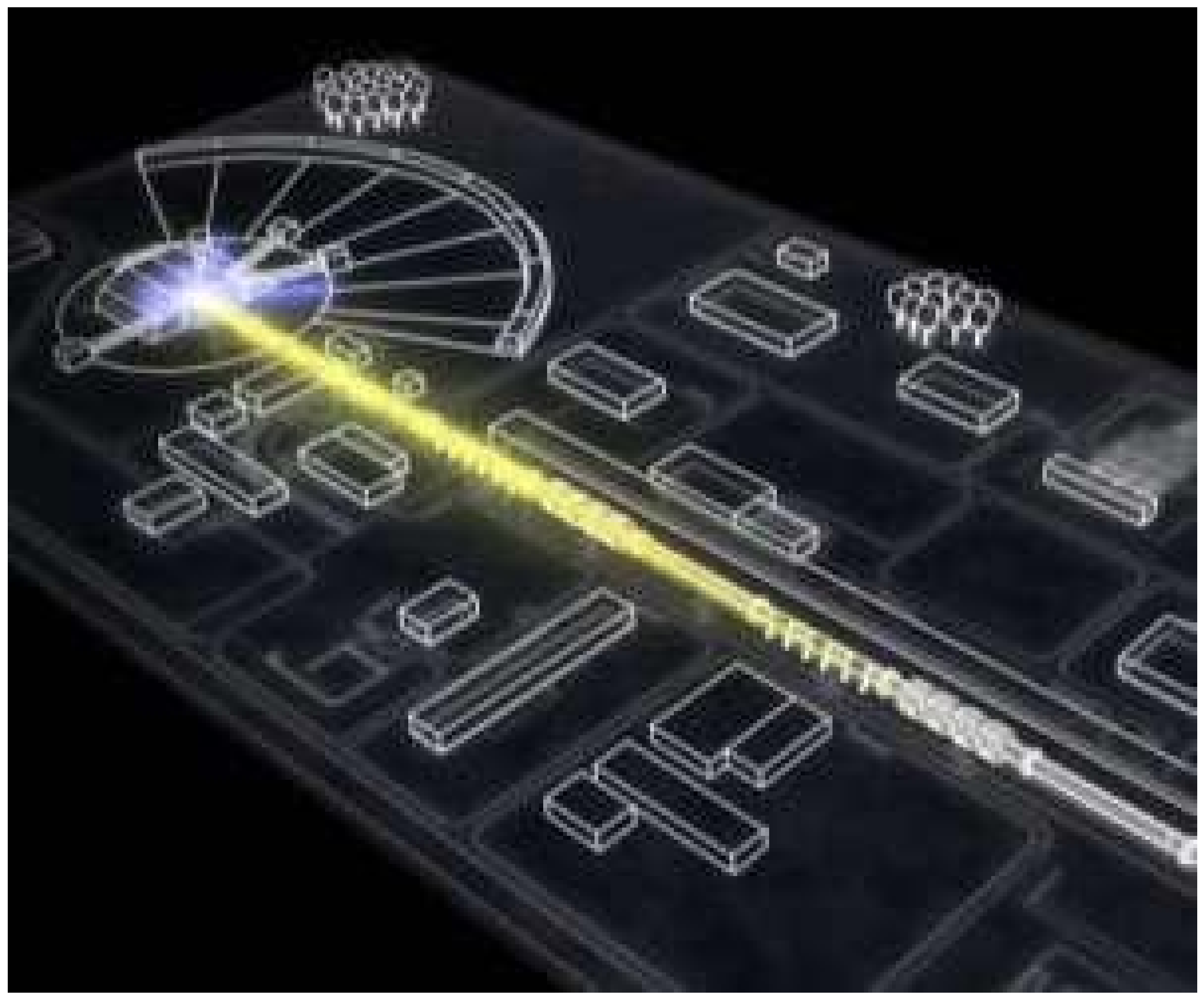
Data Management and Software

- Staff: Stig Skelboe, Thomas Rod, Lars Melvyn, (secretary) (3 FTE)
- Supporters: scientists from KU, DTU-Risø, AU

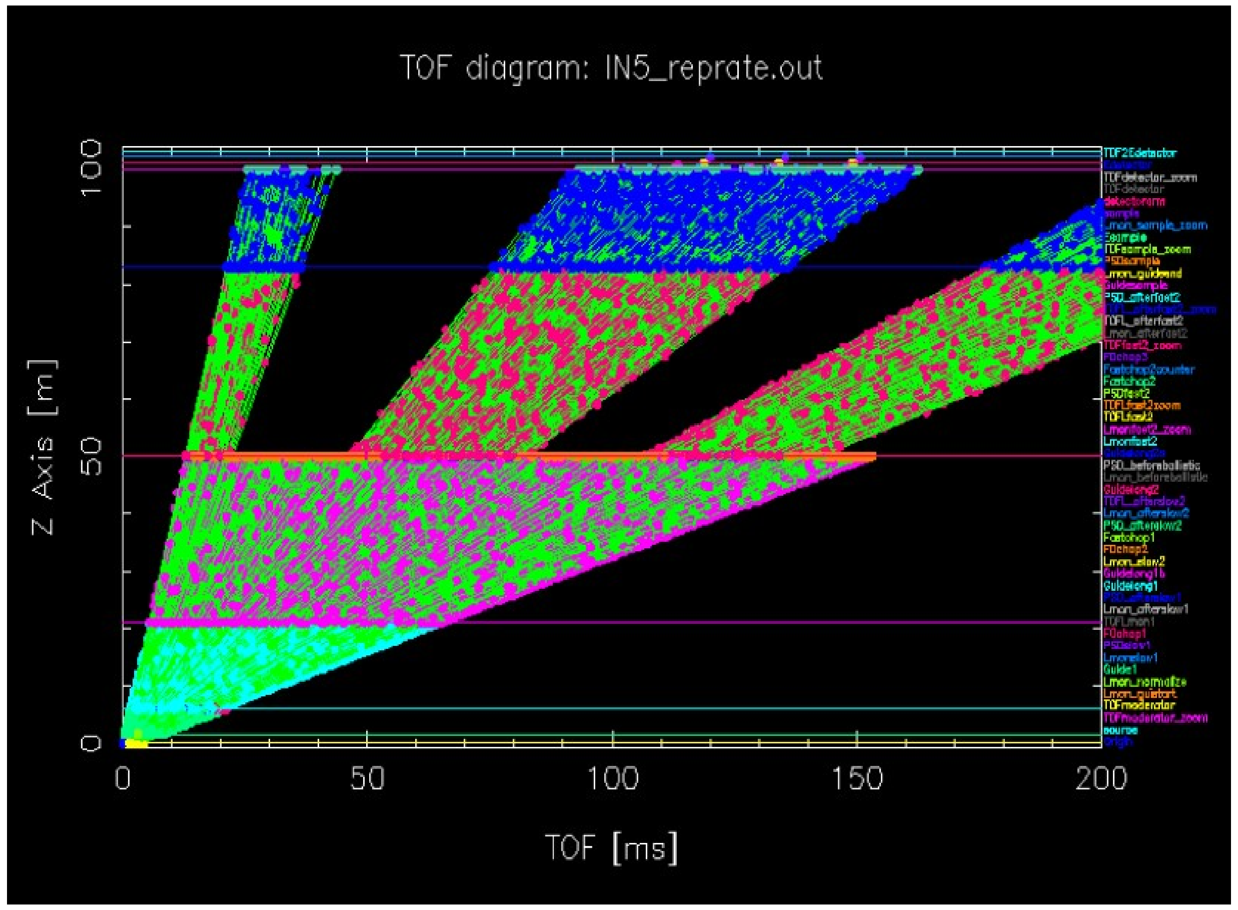
- DMSC scope (under planning)
  - User service
  - Instrument control
  - Data acquisition
  - Data archiving
  - Data visualization and analysis
  - (science modeling)
  - Instrument simulation

Instrument simulations

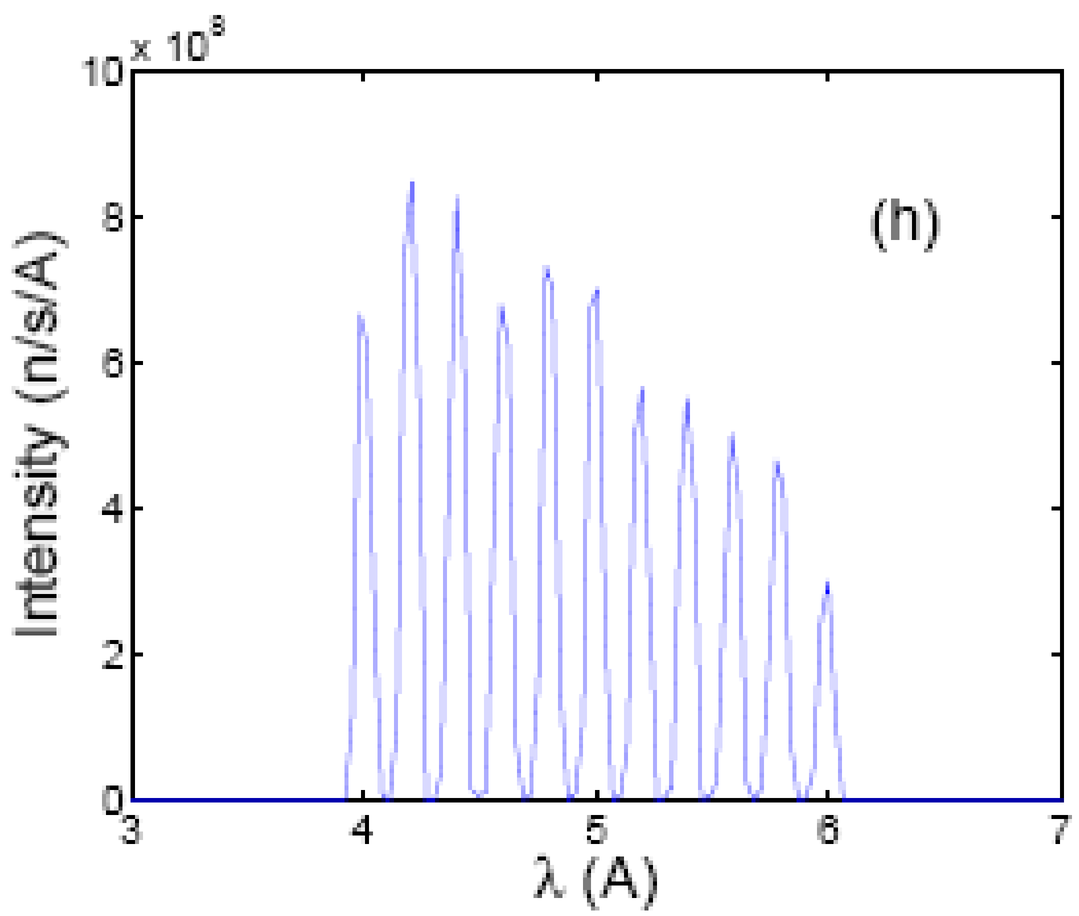
- Simulate a suite of simple instruments to investigate time structure
  - Later: move towards detailed instrument descriptions
- Answer questions from ESS instrument responsibles
  - Compare thermal powder diffraction designs
  - Compare thermal spectrometer designs
  - Analyze effect of off-specular scattering
- Prepare for virtual experiments for data analysis
  - Event mode data; bootstrap
  - Effect of the pulse tail
  - Effect of multiple scattering; sample environment
- Maintain and develop McStas
- Study guide systems
  - Long thermal guides
  - Guide bundles
  - Bi-spectral extraction
- Support function for simulators

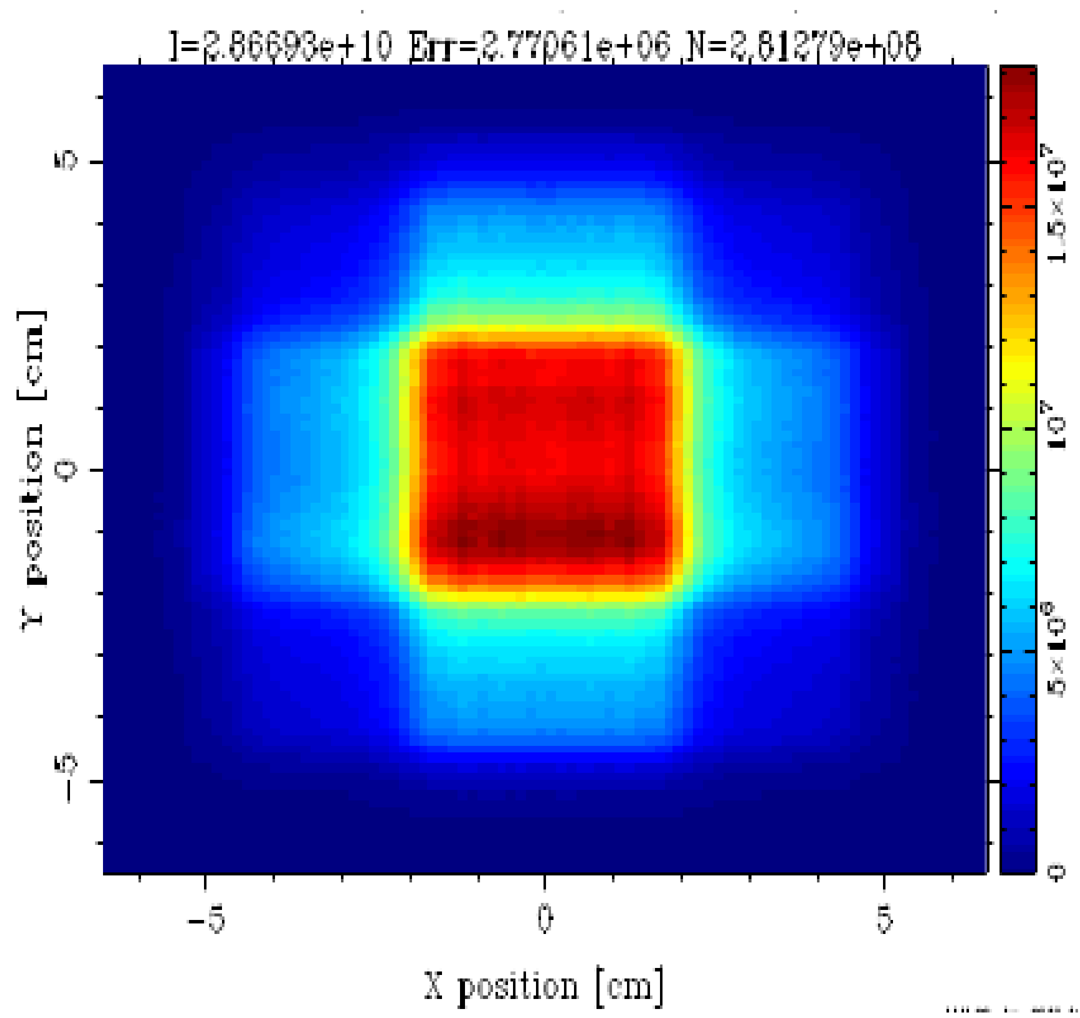


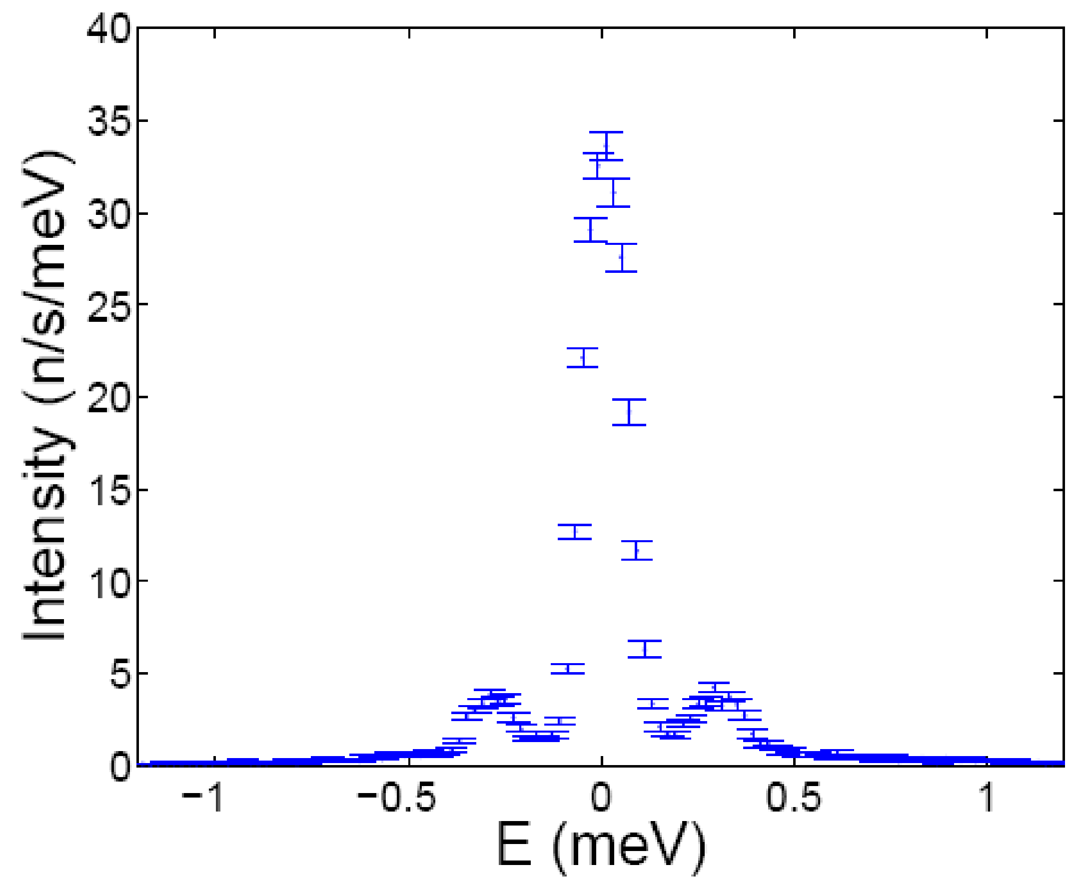
Example: Cold chopper spectrometer



- 100 m elliptical guide
- Wavelength multiplication at sample
- 30 (300) times IN5 flux
- Count rates of the order 10^8 / sec.
- VE shows expected resolution
- Moderator “Hot spot” is highly beneficial







Conclusions

- Danish universities are/will be heavy involved in many aspects of the design, construction and usage of the ESS and its instruments, including:

  → Data management
  → Radioecology
  → Instrument simulation
  → Instrument design
  → Neutron scattering experiments
  → Neutronics
  → Develop/maintain McStas

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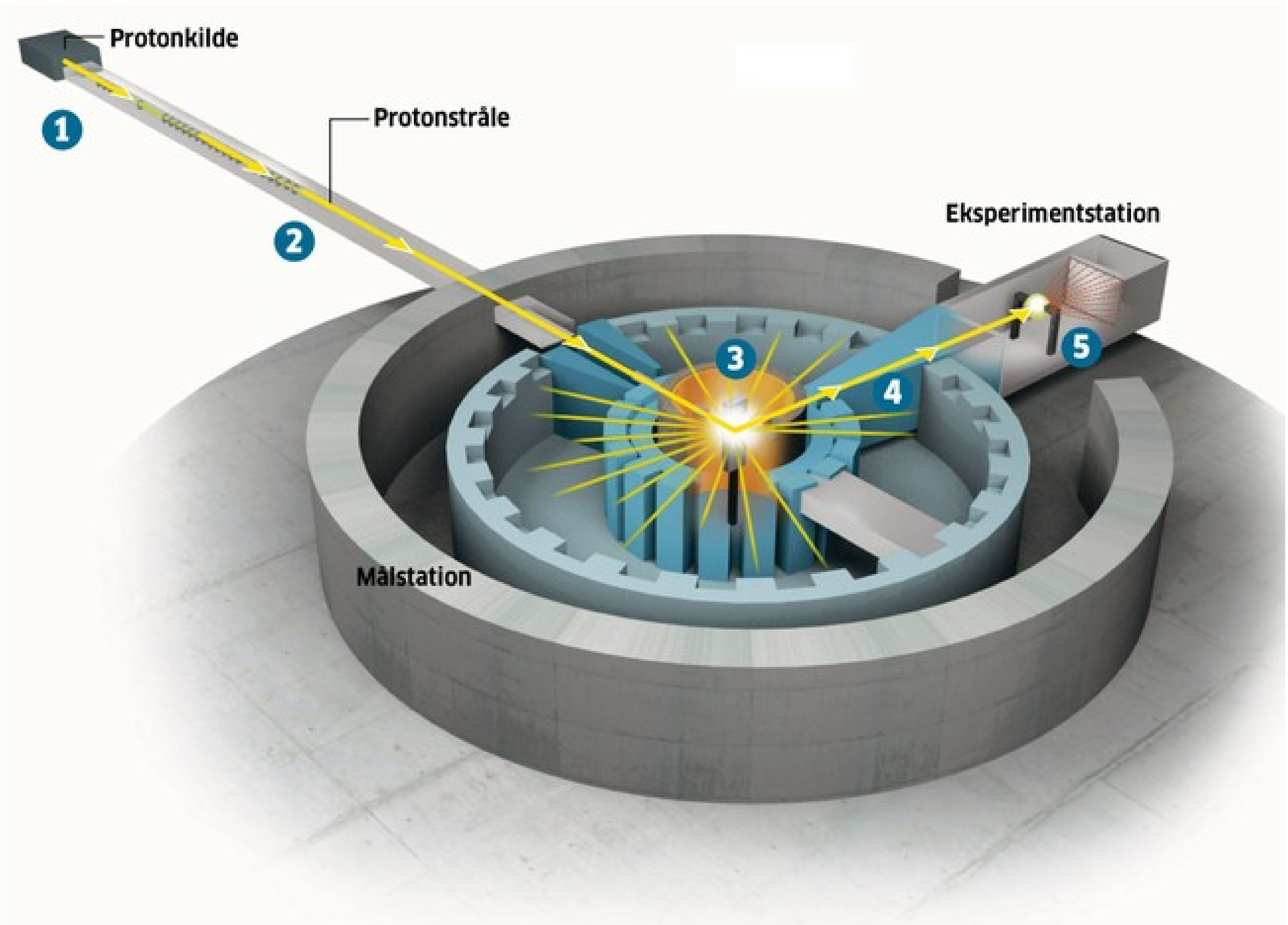
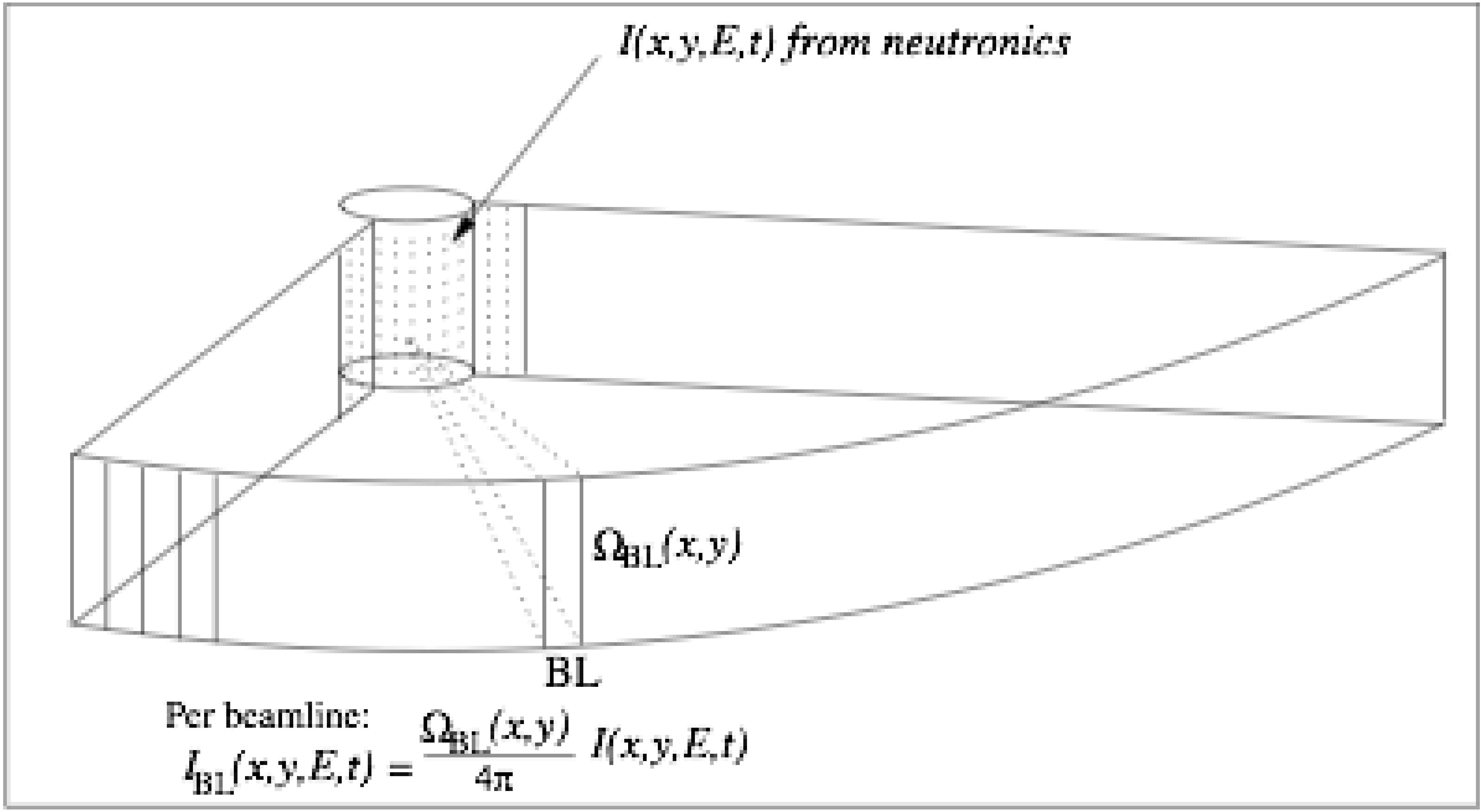
Backup slides...

Overview

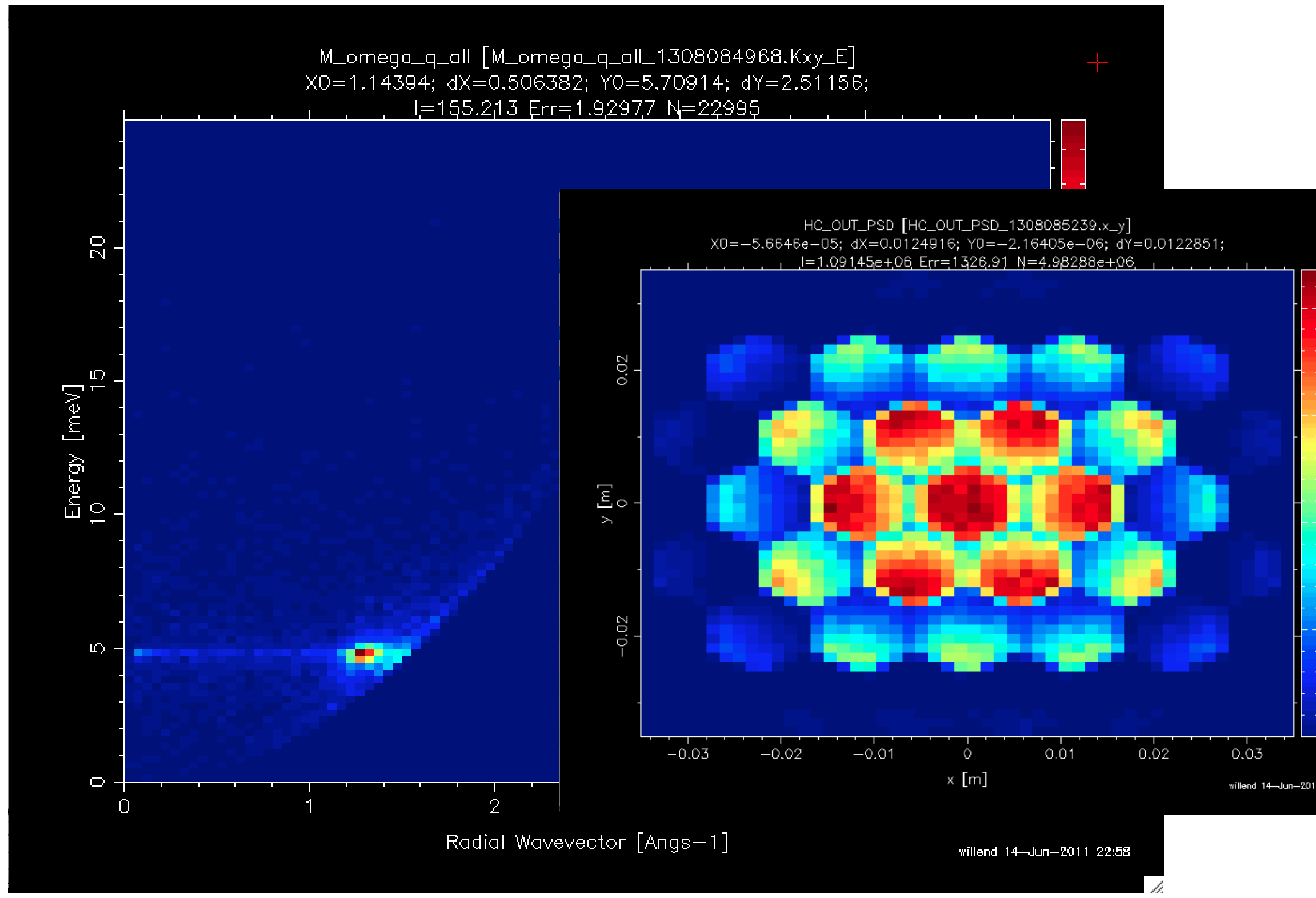

Protonkilde
1
Protonstråle
2
Eksperimentstation
3
4
5
Målstation

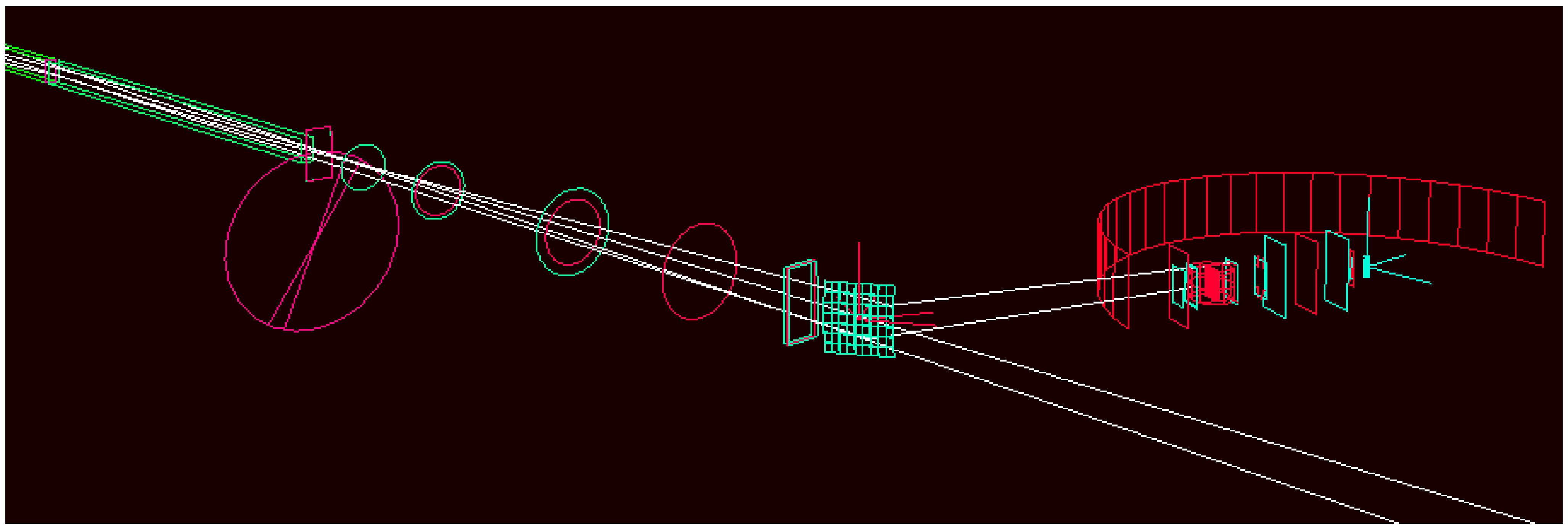
Moderators… (Where McStas starts)



Example suite: 7 TOF spectrometers:

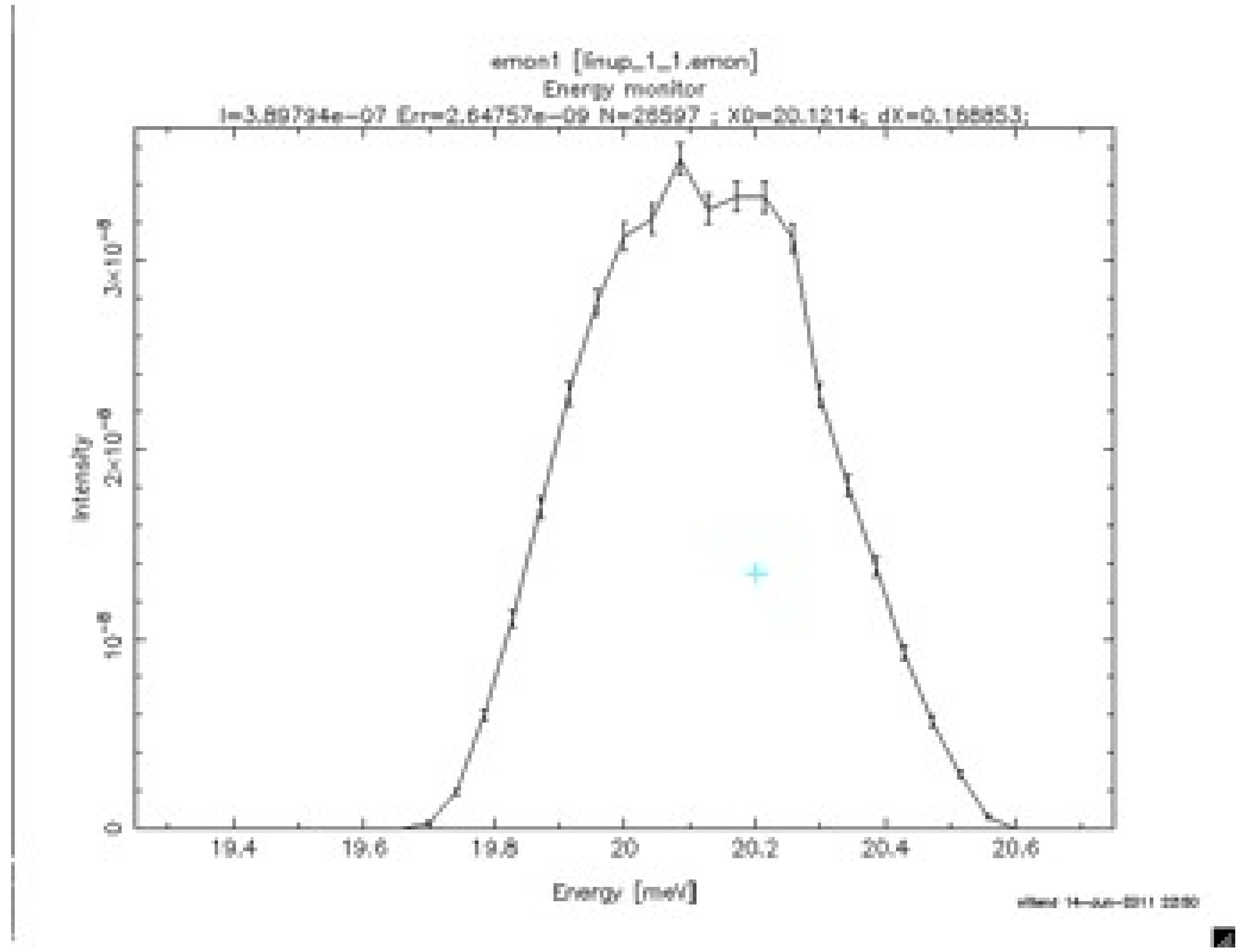
- ESS_IN5_reprate.instr
- ILL_BRISP.instr (Small-angle)
- ILL_H15_IN6.instr
- ILL_H16_IN5.instr
- ISIS_Hetfull.instr
- PSI_Focus.instr
- templateTOF.instr

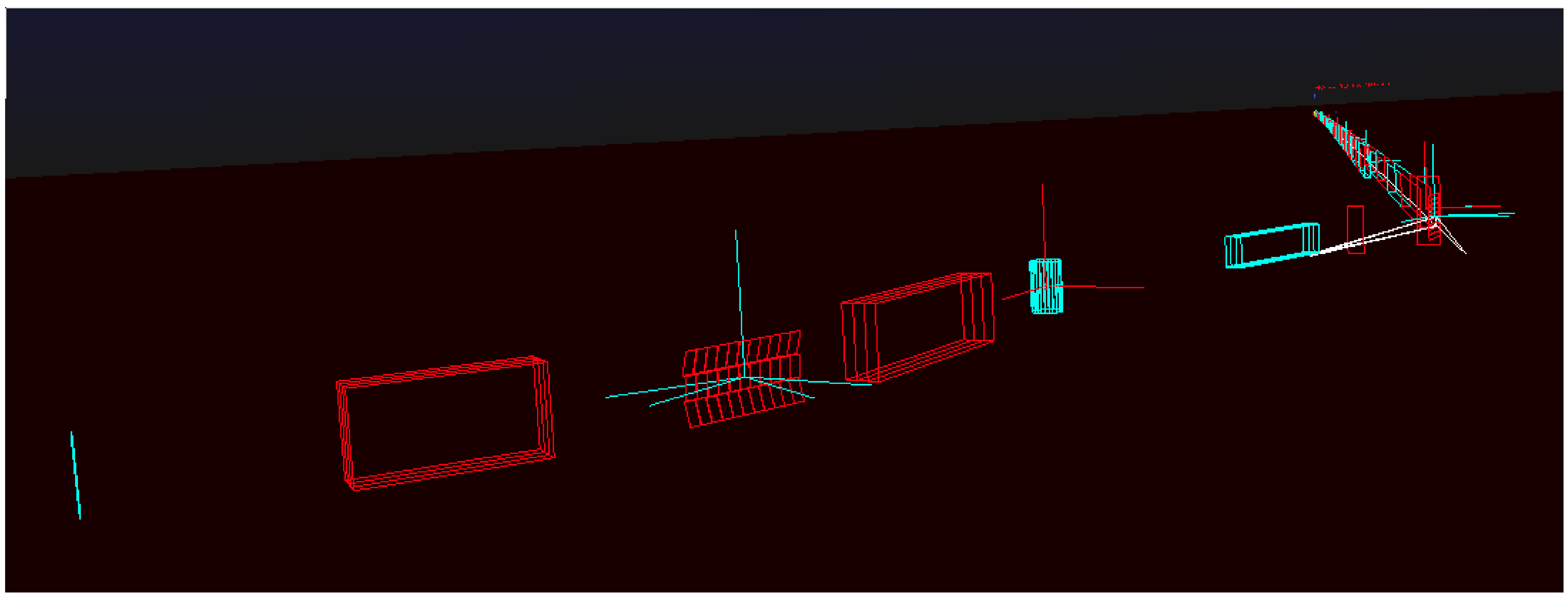




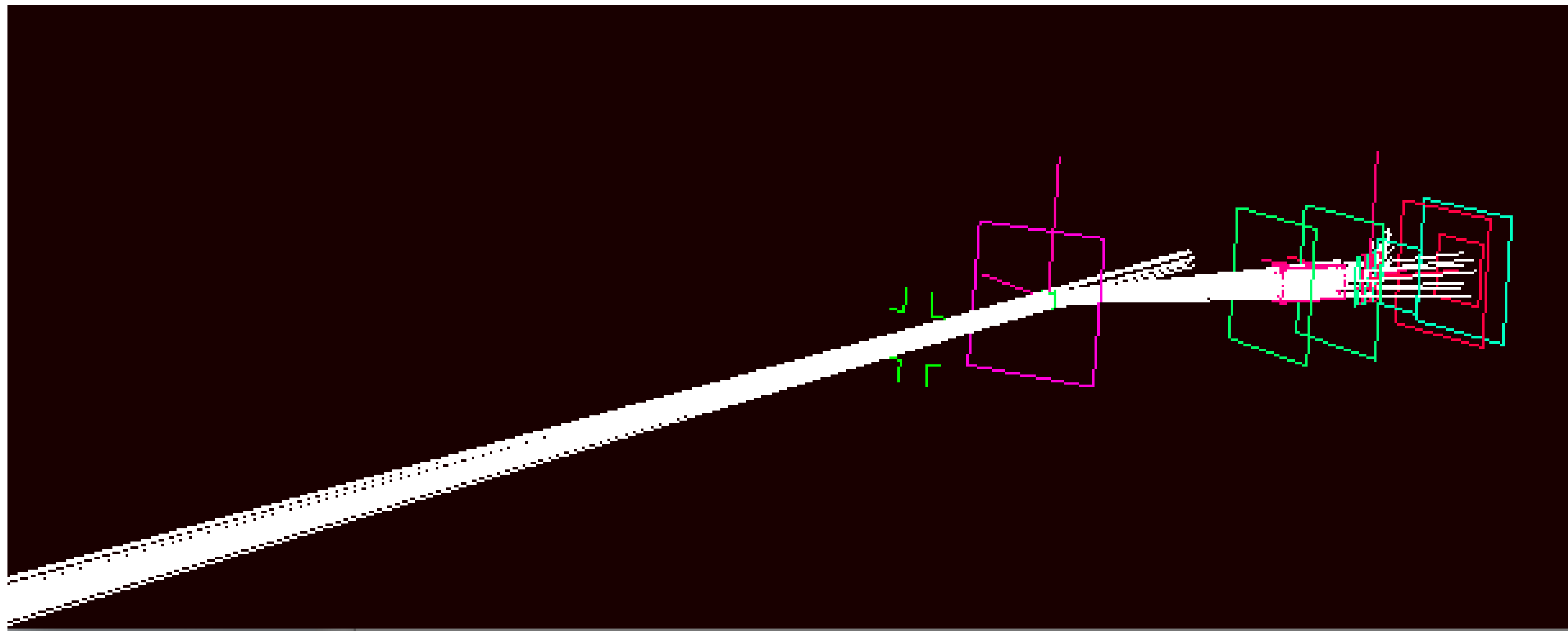
Example suite: 5 TAS

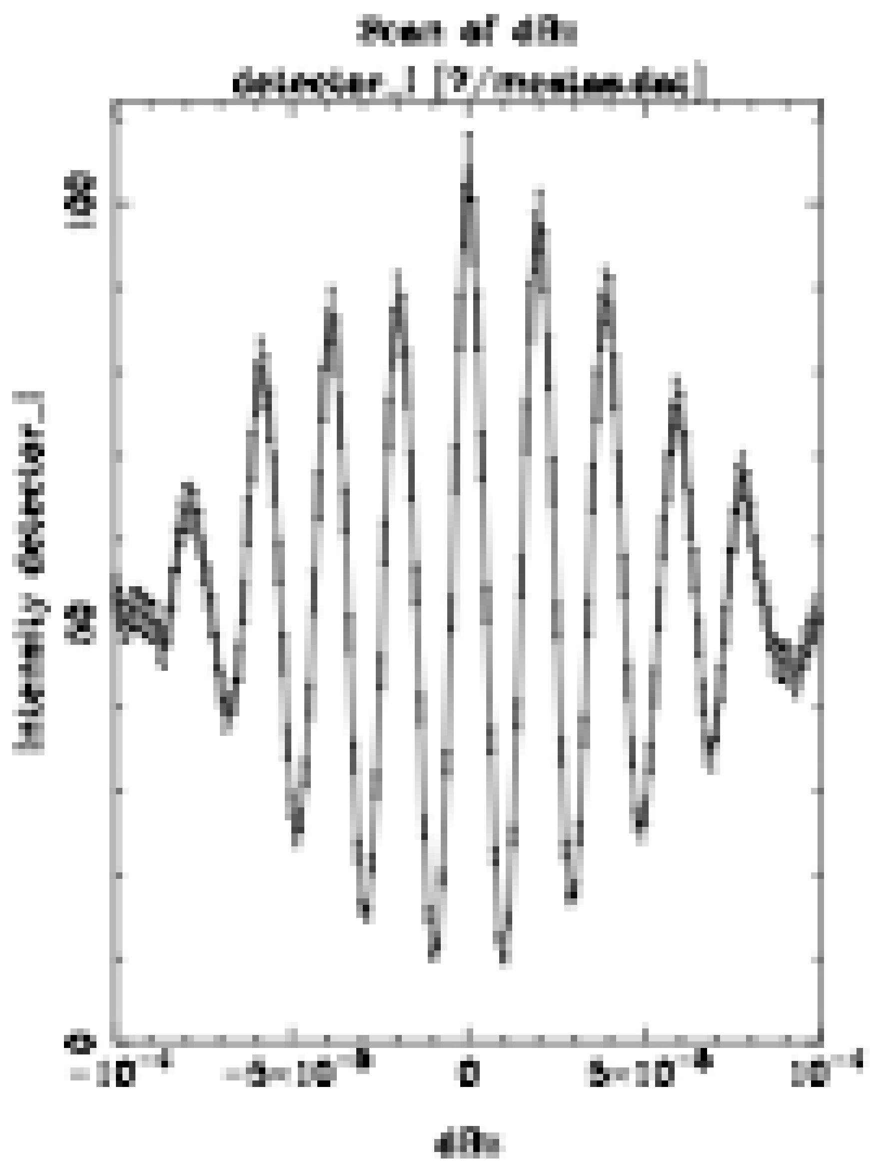
- ILL_H142_IN12.instr
- ILL_H25_IN22.instr
- h8_test.instr
- templateTAS.instr
- linup-1.instr (Risø TAS 1)
- linup-2.instr
- linup-3.instr
- linup-4.instr
- linup-5.instr
- linup-6.instr
- linup-7.instr

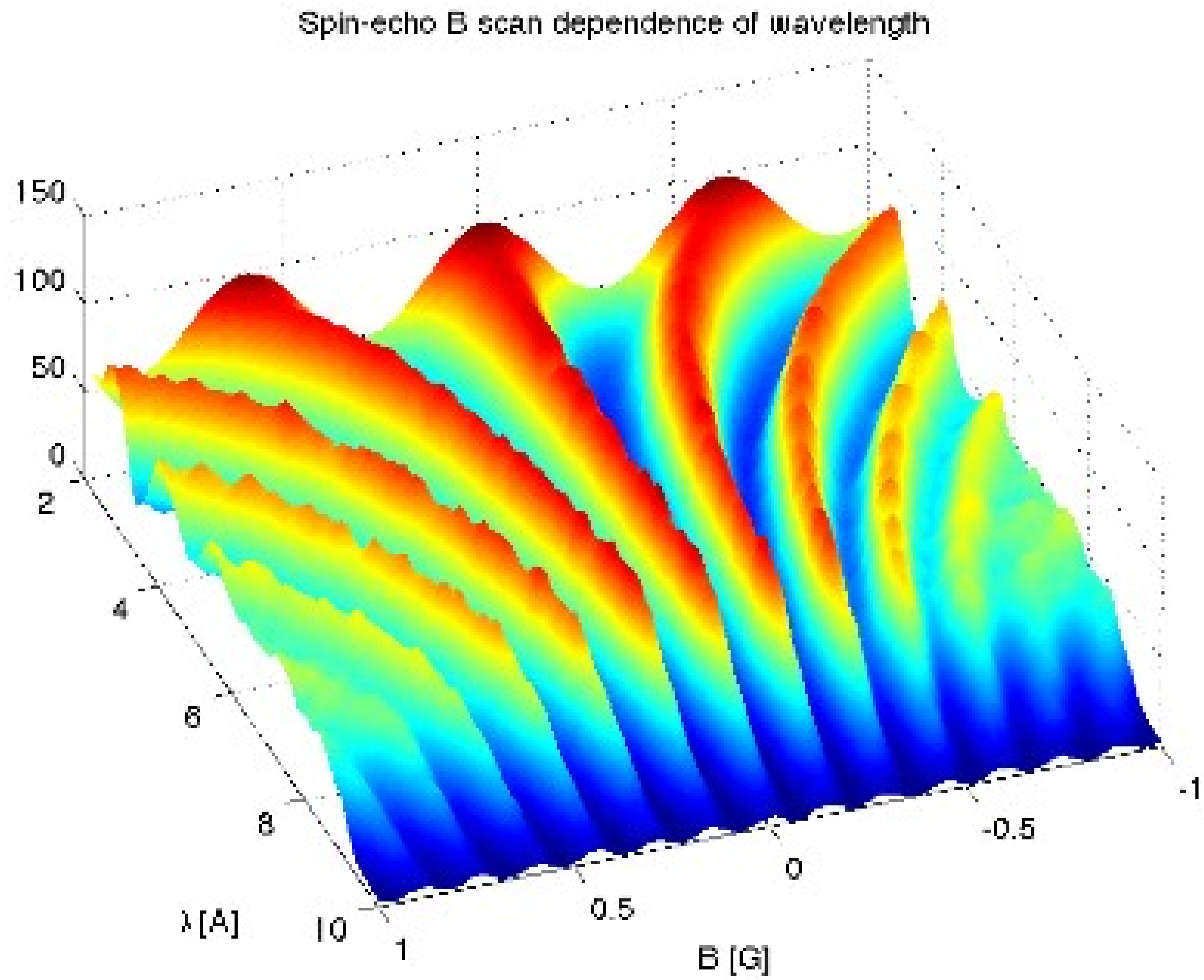




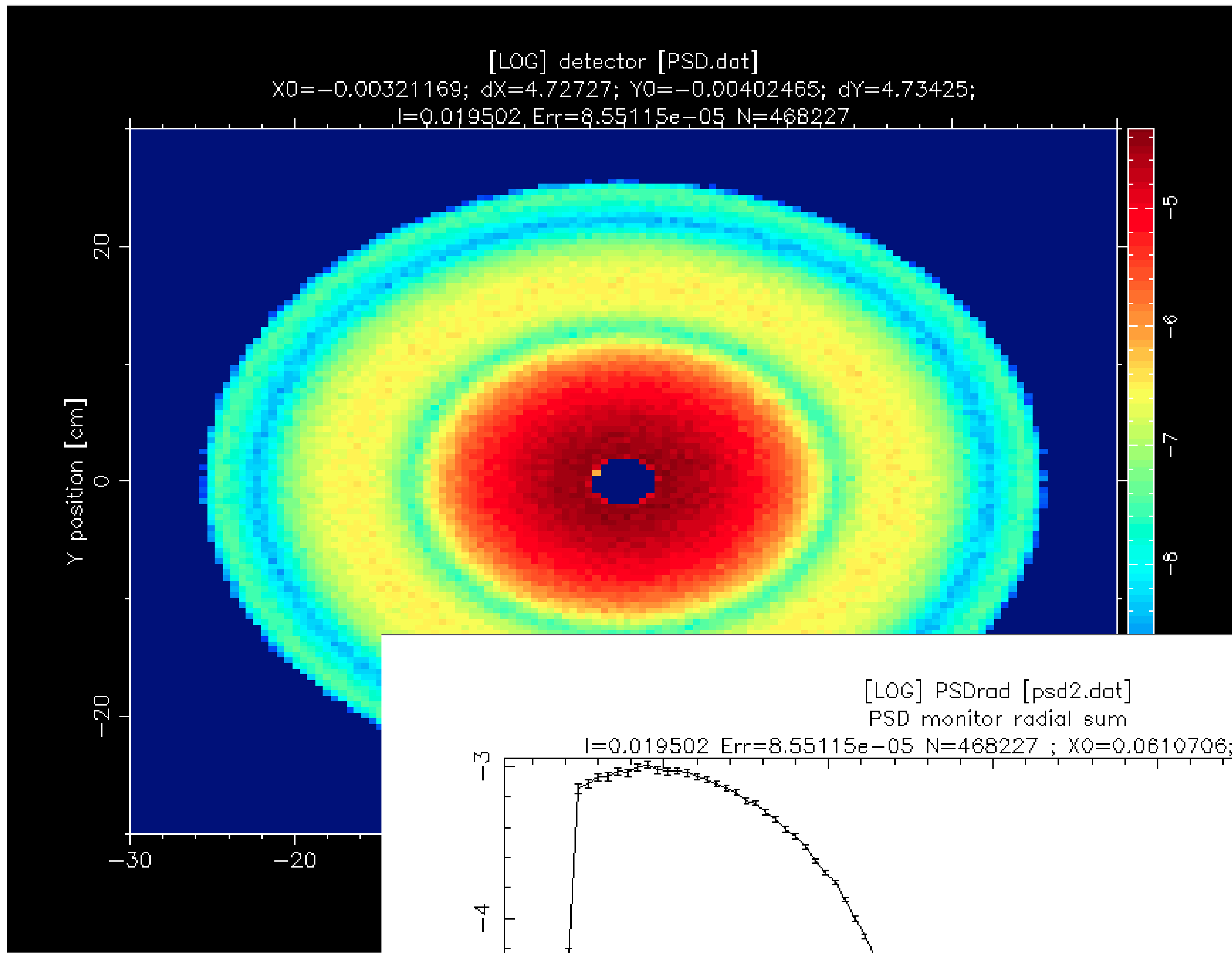
Example suite: 1 Hybrid spectrometer + 1 Spin-echo

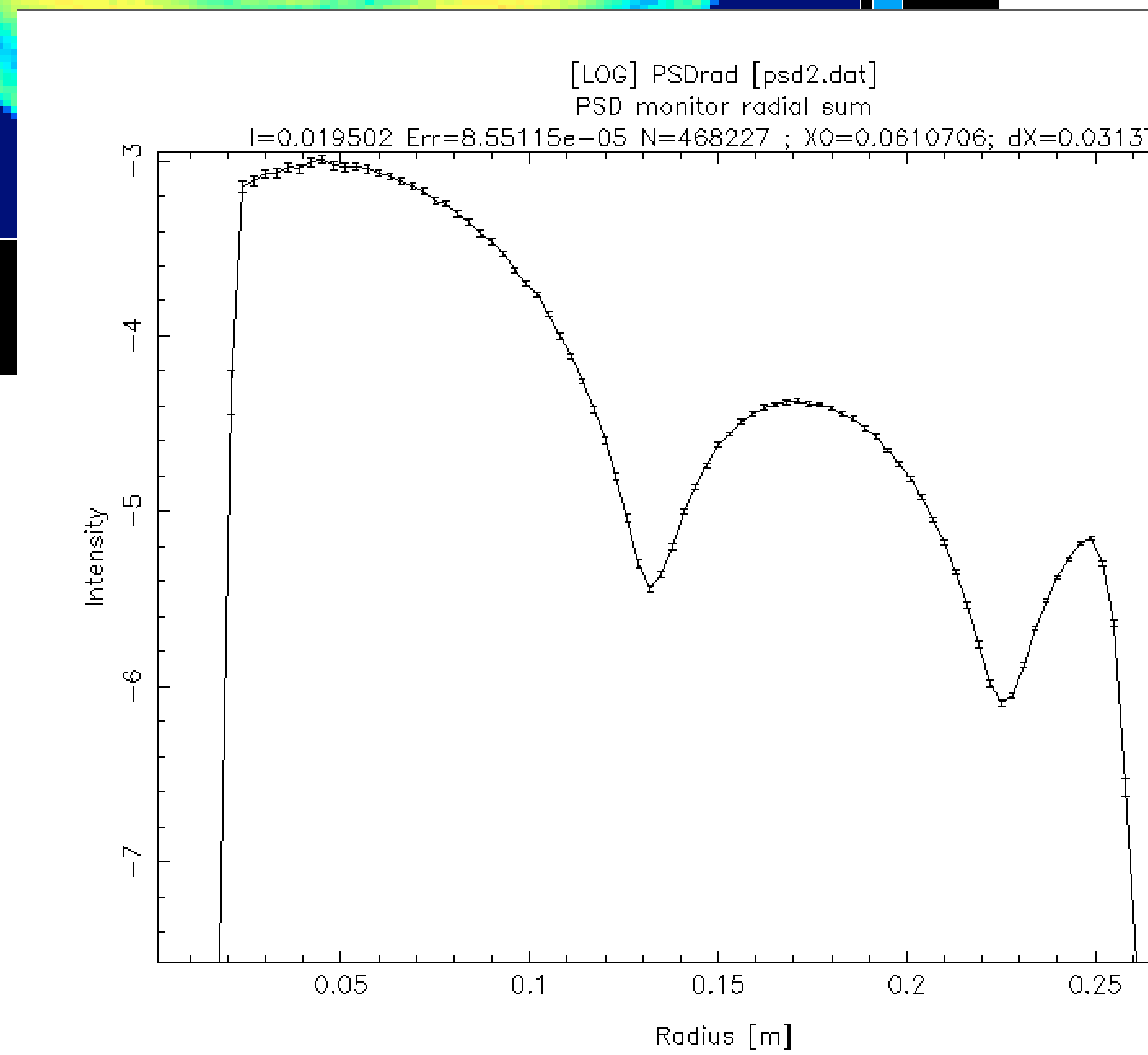


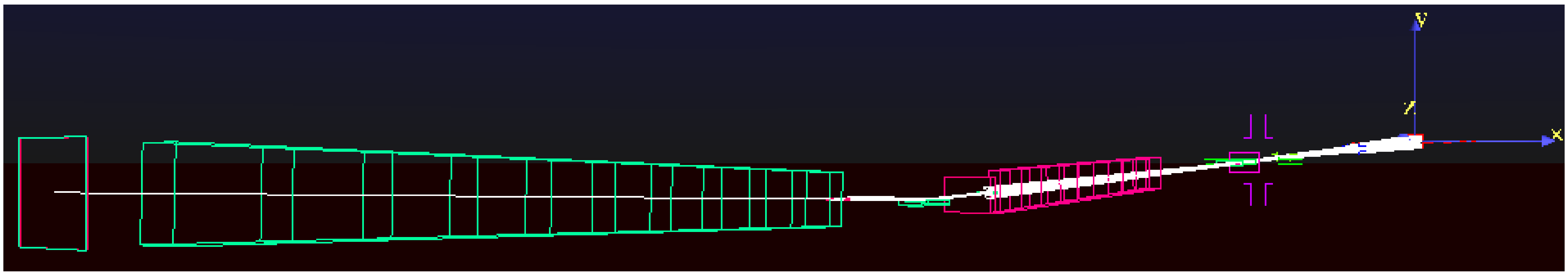




Example suite:
Large scale structures

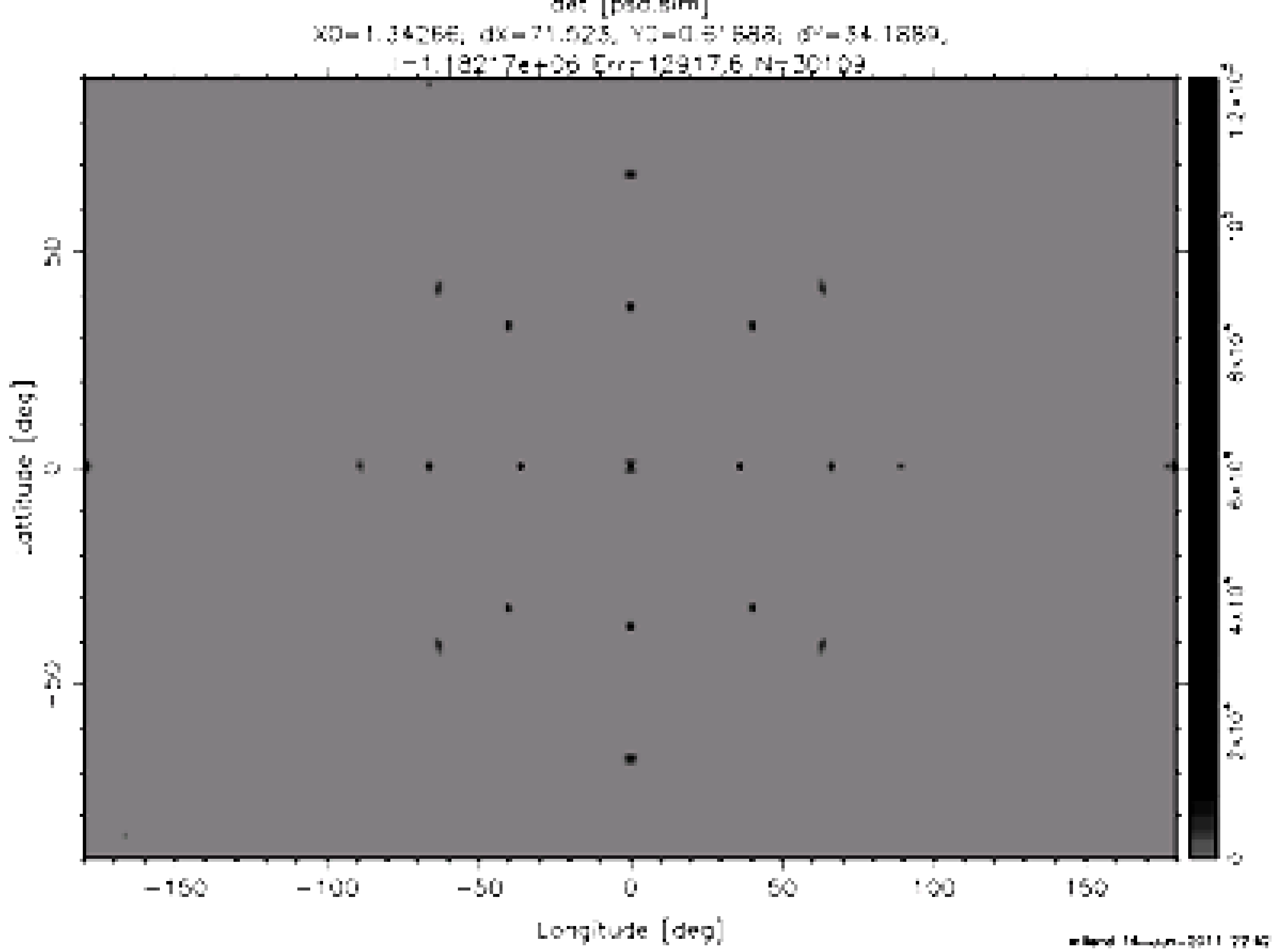


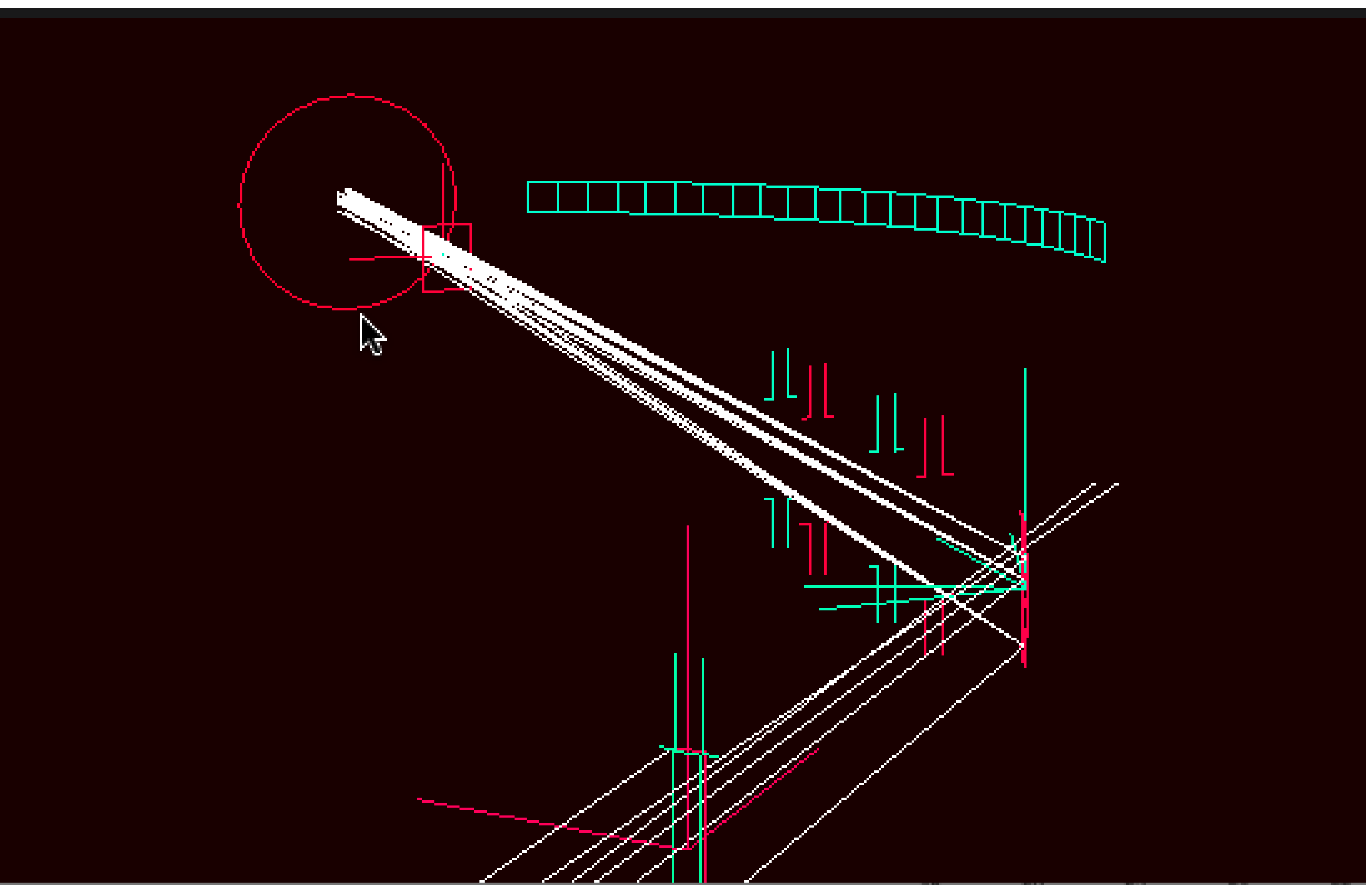


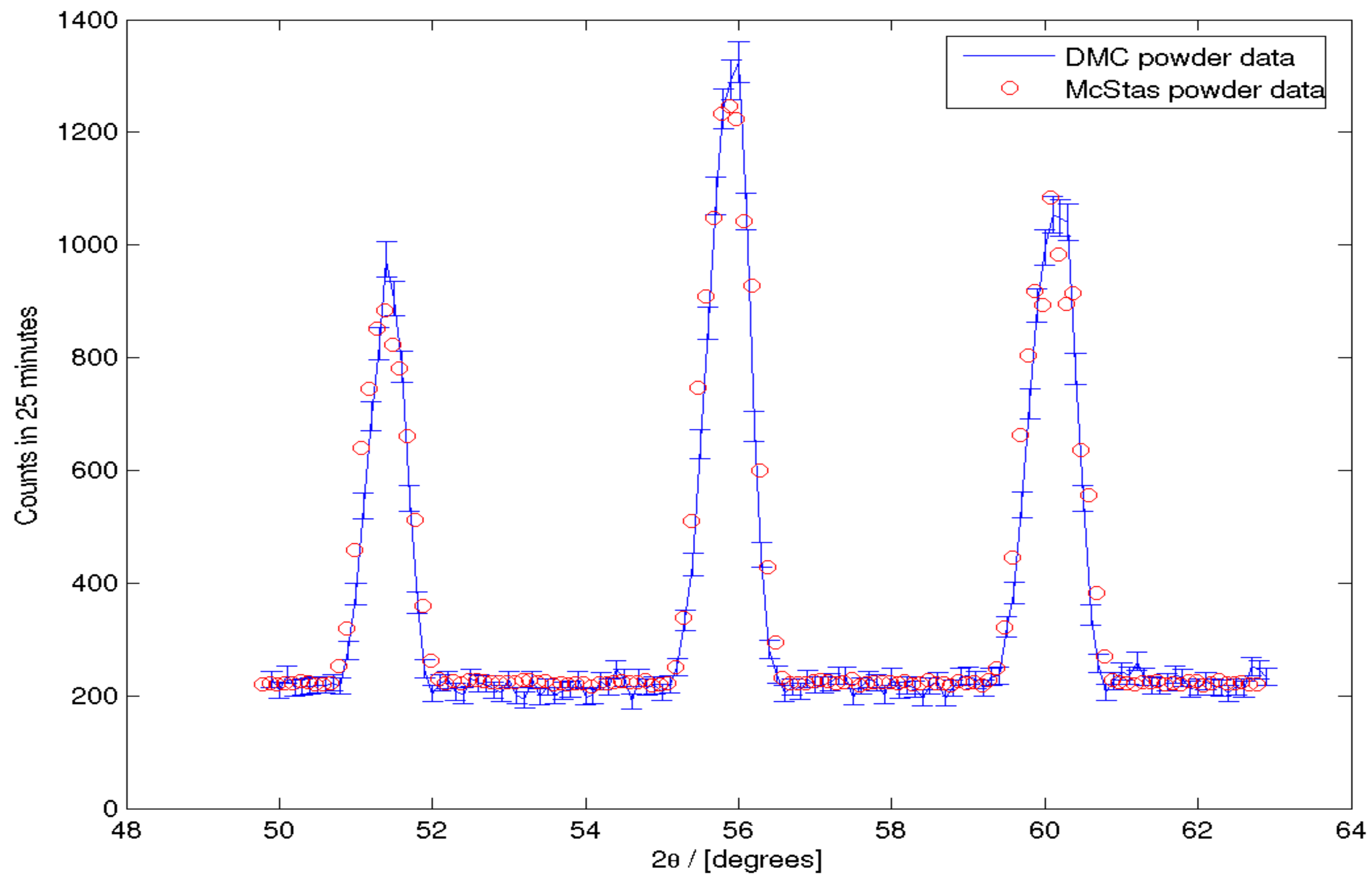


Example suite: Diffractometers

- ILL_D1A.instr
- PSI_DMC.instr
- templateDIFF.instr
- templateLaue.instr







Example suite: Imaging